A RELATIVISTIC MODEL FOR

NUCLEAR FISSION

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PREFACE

This work is a study of relativistic effects as they influence the fission of atomic nuclei. A model Hamiltonian is introduced and used to calculate energy levels of nucleons as a function of deformation. The use of this approximately relativistic Hamiltonian, together with the Strutinsky shell correction method, then enables one to estimate the magnitudes of relativistic corrections.

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CHAPTER I

INTRODUCTION

The primary goal of this work is to study relativistic effects, if any, in nuclear fission. Previous workers in the study of fission have confined themselves to non-relativistic theory, since relativistic corrections in spherical nuclei have been found by various estimates to be small. There do not appear to have been any attempts to evaluate the importance of relativistic corrections in the highly deformed nuclei which occur during fission.

In the first part of this work we discuss the relativistic covariance of the Dirac equation, and introduce potentials which apparently satisfy this covariance condition, at least in some approximation. We discuss the relativistic equivalent oscillator of Swamy (1), and the relativistic equivalent oscillator in cylindrical coordinates of Swamy and Chaffin (2). The group theory of these Hamiltonians is discussed in addition to the covariance properties. The equivalent oscillator in spherical coordinates is shown to be invariant under the Lie Algebra of $SO(4) \otimes SU(2)$, and to possess the noninvariance group $Sp(2,2) \otimes SU(2)$. This noninvariance group is further expandable to $SU(2,2) \otimes SU(2)$.

The motivation for applying the Dirac equation to the calculation of fission barriers stems from the non-spherical shapes of the nuclei during fission, and the resulting possibility of larger relativistic

corrections, as well as the results of earlier calculations which showed that relativistic corrections might be significant in heavy nuclei (3,4,5). In recent years, the method of Strutinsky (6) for calculating shell corrections to fission barriers has been discovered. This method provides a way to estimate the contribution of single particle effects in fission, and the modification of the results of the liquid drop model which would be caused by these effects. We use this method since more sophisticated calculations, such as Hartree-Fock calculations, are not yet feasible for heavy nuclei. Briefly, the Strutinsky method finds the change in the potential energy of a nucleus due to a high or low density of shell model levels near the Fermi level. A variety of potentials has been used in the various calculations of the shell model energy levels as a function of deformation. In many nuclei, the Strutinsky shell correction has been applied to show that secondary minima may occur in the potential energy surface. Shape isomers have been discovered experimentally, showing that these secondary minima do in fact exist.

The models used to calculate energy levels as a function of deformation include the harmonic oscillator shell model. The harmonic oscillator models include the one-center model of Nilsson (7), as well as the two center model based upon the Dirac equation, which corresponds to the model of Holzer, Mosel, and Greiner. One advantage of doing this is that the model can be applied for large separations of the two centers, and is asymptotically correct when the two centers separate to infinity. Hence, we can test whether or not relativistic corrections become larger at larger deformations.

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CHAPTER II

DIRAC HAMILTONIANS FOR USE AS NUCLEAR SHELL MODELS

Up to the present time the only Dirac Hamiltonian which possesses exact solutions, which reduces to an isotropic Harmonic oscillator in the non-relativistic limit, and which has been applied as a nuclear shell model is the relativistic equivalent oscillator of Swamy (1). It was introduced as a shell model by Braun and Swamy (2), who applied it to the study of electron scattering cross sections, and has been used by Swamy and Chaffin (3) to calculate relativistic corrections to Coulomb energy estimates. In this chapter, we discuss this Hamiltonian from the points of view of group theory and Lorentz invariance.

The relativistic equivalent oscillator is the Dirac Hamiltonian (in units of $\hbar = c = 1$)

$$H = \vec{\alpha}\cdot\vec{p} + \beta m_0 + i\lambda^2 \vec{\alpha}\cdot\vec{r}\,\frac{\vec{\sigma}\cdot\vec{L}+1}{|\vec{\sigma}\cdot\vec{L}+1|}$$

or

$$H = \rho_1 \vec{\sigma}\cdot\vec{p} + \rho_3 m_0 + i\lambda^2 \rho_1 \vec{\sigma}\cdot\vec{r}\,\frac{\vec{\sigma}\cdot\vec{L}+1}{|\vec{\sigma}\cdot\vec{L}+1|} \tag{1}$$

with exact solutions

$$\Phi_{\nu K\mu} = \begin{bmatrix} \sqrt{\frac{E+m_0}{2E}}\,|\nu K\mu\rangle \\ S_K \sqrt{\frac{E-m_0}{2E}}\,|\nu -K\mu\rangle \end{bmatrix} \tag{2}$$

where

$$|\nu K\mu\rangle \longrightarrow F_{\nu\ell}(r)\,\chi^{\mu}_{K}$$

$$|\nu -K\mu\rangle \longrightarrow i F_{\nu\bar{\ell}}(r)\,\chi^{\mu}_{-K} \tag{3}$$

and $F_{\nu\ell}(r)$ is the usual radial wave function for the non-relativistic harmonic oscillator, normalized so that $\int_0^\infty (F_{\nu\ell}(r))^2\, r^2\, dr = 1$.

The X^{μ}_{k} functions are the spherical spinors introduced by Biedenharn, Rose, and Arfken (4)

$$\chi^{\mu}_{K} = \sum_{\tau} C_{\mu-\tau,\tau,\mu}^{\ell(K)\ \frac{1}{2}\ j}\ \chi^{\tau}_{\frac{1}{2}}\ Y^{\mu-\tau}_{\ell(K)}(\theta,\phi) \tag{4}$$

and E is the energy eigenvalue

$$E = \sqrt{m_0^2 + 4\lambda^2(\nu + |K| + \tfrac{1}{2})} \tag{5}$$

To examine the Lorentz invariance of the above single particle equations, one should start from the general form

$$\{c\vec{\alpha}\cdot\vec{p} + \beta(m_0c^2 + U_S(\vec{r}) + \gamma^{\mu}U_{V\mu}(\vec{r}) + \gamma^5 U_{PS}(\vec{r}) + \gamma^{\mu}\gamma^5 U_{A\mu}(\vec{r}) + \sigma^{\mu\nu}U_{T\mu\nu}(\vec{r})\}\psi(\vec{r}) = E\psi(\vec{r}) \tag{6}$$

Here the $U(\vec{r})$ potentials are the scalar, vector, pseudoscalar, axial vector, and tensor type potentials of Dirac theory, and tensor type potentials of Dirac theory, and $\vec{\alpha}$, β, γ^{μ}, γ^5 and $\sigma^{\mu\nu}$ are the usual 4×4 Dirac operators.

That the above form will be Lorentz covariant may be established as Dirac did it, or as R. H. Good (5) has shown for the case of electromagnetic potentials. For that case one has the equation

$$\{\gamma^{\mu}(\frac{\partial}{\partial x^{\mu}} - ieA_{\mu}) + m_o\}\psi = 0 \qquad (7)$$

For Lorentz transformations which do not involve time reflections, the vector potential A_{μ} behaves as a vector:

$$A'_{\mu}(x') = a^{\mu}{}_{\nu} A_{\mu}(x) \qquad (8)$$

where the $a^{\mu}{}_{\nu}$ are the coefficients of the Lorentz transformation

$$x'_{\mu} = a^{\mu}{}_{\nu}\, x_{\mu}. \qquad (9)$$

The operator $\frac{\partial}{\partial x^{\mu}}$ is also a vector, i.e.

$$\frac{\partial}{\partial x'^{\mu}} = a^{\nu}{}_{\mu} \frac{\partial}{\partial x^{\nu}}. \qquad (10)$$

Now Good showed that all 4 by 4 matrices which satisfy the anticommutation relations of the γ^{μ} are equivalent up to a unitary transformation. Hence, we may choose to use the same gamma matrices in the primed frame as in the unprimed frame:

$$\{\gamma^{\mu}(\frac{\partial}{\partial x'^{\mu}} - ieA'_{\mu}(x')) + m_o\}\psi'(x') = 0 \qquad (11)$$

We require $\psi'(x')$ to be related to $\psi(x)$ by the transformation

$$\psi'(x') = \Lambda\psi(x) \qquad (12)$$

and obtain from equation (11) using the equations (8), (9), (10), and (12):

$$\left\{\left(\frac{\partial}{\partial x^{\mu}} - ie A_{\mu}(x)\right)\gamma^{\nu} a^{\mu}{}_{\nu}\,\Lambda + m_0 \Lambda\right\}\psi(x) = 0 \qquad (13)$$

And then multiplying by Λ^{-1}:

$$\left\{\left(\frac{\partial}{\partial x^{\mu}} - ie A_{\mu}(x)\right) a^{\mu}{}_{\nu}\,\Lambda^{-1}\gamma^{\nu}\Lambda + m_0\right\}\psi(x) = 0 \qquad (14)$$

so that covariance is established provided Λ satisfies the equation:

$$a^{\mu}{}_{\nu}\,\Lambda^{-1}\,\gamma^{\nu}\,\Lambda = \gamma^{\mu}. \qquad (15)$$

Good next showed that Λ matrices satisfying this condition and corresponding to Lorentz transformations do in fact exist. A similar demonstration of this was also given by Bjorken and Drell (6). Such an argument can be given for equation (5), including all of the $U(\vec{r})$ potentials, and not just the vector potentials.

To give a convincing argument that the Hamiltonian of equation (1) does not violate Lorentz covariance, one should be able to state that in a certain reference frame one of the potentials reduces to the term

$$V(\vec{r}) = i\lambda^2 \vec{q}\cdot\vec{r}\,\frac{\sigma\cdot L+1}{|\sigma\cdot L+1|} \qquad (16)$$

This reference frame should be one in which the motion of the nucleus as a whole contributes very little to the energy. To see this,

one may follow the presentation of Foldy (7). Foldy gave in this paper (reference (7)) a derivation of a many particle Hamiltonian which was consistent with Lorentz invariance up to terms of order $1/c^2$. He first started with a zero order Hamiltonian which satisfied the conditions of invariance under the Galelei group, i.e., translational, rotational, and change of reference frame invariance. For the harmonic oscillator shell model, we take this Hamiltonian to be

$$H_o = Mc^2 + \sum_i \frac{p_i^2}{2m_i} + \frac{1}{2}\sum_i m_i \omega^2 (\vec{r}_i - \vec{R})^2 \tag{17}$$

where

$$M = \sum_i m_i$$

$$\vec{R} = \sum_i \frac{m_i \vec{r}_i}{M}$$

Galelei invariance then follows from the existence of the operators:

$$\vec{P} = \sum_i \vec{p}_i \qquad \vec{S}_i = \frac{1}{2}\hbar\vec{\sigma}_i$$

$$\vec{J} = \sum_i (\vec{r}_i \times \vec{p}_i + \vec{S}_i)$$

$$\vec{K}_o = \sum_i (m_i \vec{r}_i - t\,\vec{p}_i) = M\vec{R} - t\vec{P} \tag{18}$$

which satisfy the commutation relations of the Galelei group.

Next, by requiring that the actual relativistic Hamiltonian H and change of reference frame generators $\vec{K}$ could be expanded in the forms

$$H = H_0 + H^1 + \ldots$$

$$\vec{K} = \vec{K}_0 + \vec{K}_1 + \ldots \tag{19}$$

Foldy integrated the commutation relations of the Lorentz group and obtained, up to order $1/c^2$:

$$H = Mc^2 + H^{(0)} - \frac{P^2}{2M^2c^2}U^{(0)} - \frac{P^4}{8M^3c^2} - \left(\sum_n \frac{\pi_n^2}{2m_0c}\right)\left(\frac{P^2}{2Mc}\right) + W^{(1)} \qquad (20)$$

where

$$H^{(0)} = \frac{P^2}{2M} + \sum_n \frac{\pi_n^2}{2m_n} + \frac{1}{2}m_0\omega^2 \sum_n (\vec{r}_n - \vec{R})^2$$

$$U^{(0)} = \frac{1}{2}m_0\omega^2 \sum_n (\vec{r}_n - \vec{R})^2$$

$\vec{\pi}_n$ = internal momentum of particle n

$W^{(1)}$ = a rotationally invariant function of internal variables only.

Hence, if the motion of the nucleus as a whole contributes very little to the energy, i.e.

$$\frac{P^2}{2M} \cong 0 \qquad (21)$$

Then H is given by the expression

$$H \cong \sum_n \left\{ m_nc^2 + \frac{1}{2m_n}\pi_n^2 + \frac{1}{2}m_0\omega^2(\vec{r}_n - \vec{R})^2 \right\} + W^{(1)} \qquad (22)$$

In obtaining this expression, we have not said that the value of $\vec{P}$ is zero, but merely that it is so small as to contribute very little to the energy of the nucleus. If we tried to say that it was zero, we would be subject to the type of objections, based on the uncertainty principle, which were raised by Eddington (8), (10) and answered by Dirac, Peierls, and Pryce (9).

The above results show that it is possible to consider the total energy of the nucleus as being given by the sum of the single particle energies of nucleons moving in a harmonic oscillator well. One can, therefore, describe each nucleon as moving according to a Dirac equation, and use this Dirac equation to obtain single particle energies. One should note that in writing down equation (6) we have used $\vec{p}$, the momentum of the particle with respect to a reference frame fixed in space, and not $\vec{\pi}$, the momentum with reference to the center of mass, in accordance with reference (11).

By a slight modification of some arguments due to Miller (12), we would now like to show that the potential of the above equation (16) can be classified as a vector potential.

One first requires that the relativistic parity

$$P = \gamma^0 P_{NR} = \beta P_{NR} \tag{23}$$

(here P_{NR} is the operation $\vec{r} \to -\vec{r}$) and total angular momentum

$$\vec{J} = \vec{L} + \frac{1}{2}\vec{\sigma} \tag{24}$$

should commute with the Hamiltonian of equation (6). This leads to some restrictions on the angle dependence of the potentials $U(\vec{r})$. We first put

$$\vec{L} = \vec{r} \times \vec{p} = -i[\hat{\phi}\frac{\partial}{\partial\theta} - \hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}] \tag{25}$$

and

$$\vec{\sigma} = \hat{r}\begin{pmatrix} \cos\theta & \sin\theta\, e^{-i\phi} \\ \sin\theta\, e^{i\phi} & -\cos\theta \end{pmatrix} + \hat{\theta}\begin{pmatrix} -\sin\theta & \cos\theta\, e^{-i\phi} \\ \cos\theta\, e^{i\phi} & \sin\theta \end{pmatrix}$$
$$+ \hat{\phi}\begin{pmatrix} 0 & -ie^{-i\phi} \\ ie^{i\phi} & 0 \end{pmatrix} \tag{26}$$

where $\hat{r}$, $\hat{\theta}$, $\hat{\phi}$ are the unit vectors of the spherical coordinate system.

Using the metric in which the zeroth component is positive, one can write the vector potential as

$$\gamma^{\mu} U_{V_\mu}(\vec{r}) = \gamma^0 U_V^0(\vec{r}) - \vec{\gamma}\cdot\vec{U}_V(\vec{r}) \tag{27}$$

From the required commutation of $\vec{J}$ and P with the above interaction, we find that $\vec{U}_v$ should be of the form

$$\vec{U}_v(\vec{r}) = \hat{r}\, U_v^r(r) \tag{28}$$

where $U_v^r(r)$ is independent of angle.

At this point in these arguments one should consider the form of our proposed potential of equation (16):

$$V(\vec{r}) = i\lambda^2 \vec{\alpha}\cdot\vec{r}\,\frac{\sigma\cdot L+1}{|\sigma\cdot L+1|} = i\lambda^2 \rho_1 \vec{\sigma}\cdot\hat{r}\, r\,\frac{\sigma\cdot L+1}{|\sigma\cdot L+1|}$$
$$= i\lambda^2 \beta\vec{\gamma}\cdot\hat{r}\, r\,\frac{\sigma\cdot L+1}{|\sigma\cdot L+1|} \tag{16}$$

so that one apparently has a vector potential with

$$U_V^r(r) = r\,\frac{\sigma\cdot L+1}{|\sigma\cdot L+1|} \tag{29}$$

One can, in fact, show that the parity and total angular momentum operators do commute with the potential of equation (16).

After the arguments which led to the form of equation (28), Miller considered Hermiticity requirements. In the cases considered by Miller, this leads to the condition that

$$U_v{}^r(r)^* = U_v{}^r(r)$$

or that $U_v{}^r(r)$ is real. In our case, however, the inclusion of the operator $\frac{\sigma\cdot L + 1}{|\sigma\cdot L + 1|}$ in the potential, plus the anticommutation relation:

$$\left[\frac{\sigma\cdot L+1}{|\sigma\cdot L+1|}, \vec{\sigma}\cdot\vec{r}\right]_+ = 0 \qquad (30)$$

leads to the opposite conclusion, that $U_v{}^r(r)$ should be pure imaginary. We, therefore, conclude that the potential of equation (16), (which is pure imaginary when operating on a solution $\phi_{vK\mu}$) satisfies Hermiticity and hence is not at variance with probability conservation.

To summarize, we can reason that the potential of equation (16) is consistent with the requirements of Lorentz covariance provided we consider it to arise in a reference frame in which

$$U_v^0(\vec{r}) = 0$$
$$\vec{U}_v(\vec{r}) = (i\lambda^2 r)\hat{r}\,\frac{\sigma\cdot L+1}{|\sigma\cdot L+1|} \qquad (31)$$

so that

$$\beta\gamma^\mu U_{v\mu}(\vec{r}) = i\lambda^2\rho_1\,\vec{\sigma}\cdot\vec{r}\,\frac{\sigma\cdot L+1}{|\sigma\cdot L+1|} \qquad (32)$$

Having considered the Hamiltonian of equation (1) from the point of view of Lorentz covariance, we would now like to consider its group structure. This analysis was done by Chaffin (13), (14), who showed that operators existed satisfying the Lie Algebra of $SO(4) \otimes SU(2)$ and commuting with the Hamiltonian of equation (1). Furthermore, it was shown that this Lie algebra can be enlarged to $SO(4,1) \times SU(2)$. In this thesis we would like to point out that this Lie Algebra can be further enlarged to $SU(2,2) \otimes SU(2)$, where $SU(2,2)$ is isomorphic to the group which is familiarly known as the conformal group.

The group $SO(4)$ is the group of real 4×4 orthogonal matrices with determinant plus one. The Lie algebra consists of six operators $\vec{M}$ and $\vec{J}$ satisfying the commutation relations

$$\begin{aligned} [M_k, M_\ell] &= i \varepsilon_{k\ell m} J_m \\ [J_k, J_\ell] &= i \varepsilon_{k\ell m} J_m \\ [J_k, M_\ell] &= i \varepsilon_{k\ell m} M_m \end{aligned} \tag{33}$$

In the case of the realization of this Lie Algebra as a set of operators commuting with the Hamiltonian of equation (1), the $\vec{J}$ operators are simply the total angular momentum operators

$$\vec{J} = \vec{L} + \frac{1}{2} \vec{\sigma} \tag{34}$$

so that the Hamiltonian is rotationally invariant. The $\vec{M}$ operators have the form

$$\vec{M} = \frac{-i\sqrt{\frac{H^2-m_0^2}{4\lambda^2}+|K|-\frac{1}{2}}}{2\lambda(2|K|-1)}\ \frac{1}{2}\left[(\vec{\Omega}+\vec{\Omega}^+)+\frac{K}{|K|}(\vec{\Omega}^+-\vec{\Omega})\right]$$
$$+\frac{1}{2}i\left[(\vec{\Omega}+\vec{\Omega}^+)+\frac{K}{|K|}(\vec{\Omega}-\vec{\Omega}^+)\right]\frac{\sqrt{\frac{H^2-m_0^2}{4\lambda^2}+|K|-\frac{1}{2}}}{2\lambda(2|K|-1)}$$
$$-\frac{1}{2}\ \frac{H^2-m_0^2}{4\lambda^2(|K|-\frac{1}{2})(|K|+\frac{1}{2})}\vec{J} \tag{35}$$

$$\vec{\Omega} = \left[\vec{\sigma}\cdot\vec{p} - i\lambda^2\vec{\sigma}\cdot\vec{r}\,\frac{\sigma\cdot L+1}{|\sigma\cdot L+1|}\right]\vec{\sigma}\times\vec{L} \tag{36}$$

This $\vec{M}$ operator is an operator which converts one state $\phi_{\nu k\mu}$ of a given energy level into a linear combination of states $\phi_{\nu'k'\mu'}$ of the same energy level. It was constructed in two steps: (1) first finding the matrix elements of $\vec{\Omega}$, and (2) second constructing an operator which depends on $\vec{\Omega}$, $\vec{\Omega}^+$ and $\vec{J}$ and has the correct matrix elements for the $\vec{M}$ operators of the SO(4) group. These latter matrix elements were determined by Pauli (15).

The $\vec{M}$ operator is responsible for the high degree of degeneracy (higher than the $2j+1$ fold degeneracy of the rotation group) which the Hamiltonian possesses. This degeneracy is given by

$$d = 2(n+1)(n+2) \tag{37}$$
$$n = 0,1,2,\ldots$$

A factor of two in this degeneracy is accounted for by a degeneracy with respect to the sign of kappa, as we can see from equation (5). This is

where we get the SU(2) subgroup of the invariance group SO(4) ⊗ SU(2). The operators corresponding to this SU(2) are given by

$$X_1 = \frac{1}{\sqrt{H^2 - m_0^2}}\,\vec{\sigma}\cdot\vec{b}$$
$$X_2 = i X_1 \rho_3 \frac{\sigma\cdot L + 1}{|\sigma\cdot L + 1|} \tag{38}$$
$$X_3 = \rho_3 \frac{\sigma\cdot L + 1}{|\sigma\cdot L + 1|}$$

where

$$\sigma\cdot b = \sigma\cdot p + i\lambda^2\,\sigma\cdot r\,\frac{\sigma\cdot L + 1}{|\sigma\cdot L + 1|}$$

and

$$x_1\,\phi_{\nu\kappa\mu} = S_k\,\phi_{\nu\,-\kappa\mu} \tag{39}$$

$$S_\kappa = \text{sign of kappa}$$

The above $\vec{X}$ operators commute with H, $\vec{M}$, and $\vec{J}$, as they should to form the SU(2) part of the Lie algebra of the SO(4) ⊗ SU(2) invariance group.

If we consider operations which convert a state function of one energy level into linear combinations of other energy levels, and try to enlarge the Lie algebra of the invariance group to include this type of non-invariant operator, it is possible to find the Lie algebra of SO(4,1) ⊗ SU(2). One obtains the operator

$$T = \frac{1}{4\lambda}\left[\sqrt{\frac{H^2-m_0^2}{4\lambda^2}+|K|-\frac{1}{2}}\;\frac{\sigma\cdot b}{\sqrt{H^2-m_0^2}}\,\sigma\cdot a + \sigma\cdot a\,\frac{\sigma\cdot b}{\sqrt{H^2-m_0^2}}\sqrt{\frac{H^2-m_0^2}{4\lambda^2}+|K|-\frac{1}{2}}\right]\frac{1}{2}\left(1+\frac{K}{|K|}\right)$$

$$+\frac{1}{4\lambda}\left[\sqrt{\frac{H^2-m_0^2}{4\lambda^2}+|K|-\frac{1}{2}}\;\sigma\cdot a\,\frac{\sigma\cdot b}{\sqrt{H^2-m_0^2}} + \frac{\sigma\cdot b}{\sqrt{H^2-m_0^2}}\,\sigma\cdot a\sqrt{\frac{H^2-m_0^2}{4\lambda^2}+|K|-\frac{1}{2}}\right]\frac{1}{2}\left(1-\frac{K}{|K|}\right) \tag{40}$$

where $$\sigma\cdot a = \sigma\cdot p - i\lambda^2\,\sigma\cdot r\,\frac{\sigma\cdot L+1}{|\sigma\cdot L+1|}$$

in addition to the operators

$$\vec{N} = -i[\vec{M},T] \tag{41}$$

These operators complete the Lie algebra of $SO(4,1)$, and allow the non-invariance group $SO(4,1) \otimes SU(2)$ to be formed.

All of the above group theory of the oscillator Hamiltonian of equation (1) was presented in the author's MS thesis. We would like to point out the possibility of a further enlargement of the non-invariance group.

One should first, however, make note of the following isomorphisms

$$\begin{aligned} SO(4) &\tilde{=} (SU(2) \otimes SU(2))/Z_2 \\ SO(4,1) &\tilde{=} Sp(2,2)/Z_2 \\ SO(4,2) &\tilde{=} SU(2,2)/Z_2 \end{aligned} \tag{42}$$

These isomorphisms can be demonstrated by using the methods of Talman (16) or Esteve and Sona (17). They become particularly relevant when

one considers the actual representations realized by the solutions of the Hamiltonian of equation (1). These representations correspond to $(j_1, j_2) = (0, \frac{1}{2}), (\frac{1}{2}, 1), (\frac{1}{2}, 1), (1, \frac{3}{2}), \ldots$ where j_1 and j_2 are defined by the eigenvalues of the SO(4) Casimir invariants:

$$C(1) \to j_2(j_2 + 1)$$
$$C(2) \to j_1(j_1 + 1) \tag{43}$$

where
$$C(1) = \frac{1}{2}\left(\vec{M}\cdot\vec{M} + \vec{J}\cdot\vec{J}\right) = \frac{1}{2}\left[\frac{(H^2 - m_0^2)^2}{16\lambda^4} - \frac{3}{4}\right]$$
$$C(2) = \vec{J}\cdot\vec{M} = \frac{1}{2}\left[\frac{H^2 - m_0^2}{4\lambda^2}\right] \tag{44}$$

and hence

$$j_1 = \frac{V + |K| - 1}{2}, \qquad j_2 = \frac{V + |K|}{2} \tag{45}$$

Since j_1 is integral when j_2 is half integral, we are considering double valued representations of SO(4) (see Talman, reference (16)). Hence it is a little more accurate to call the invariance group as $(SU(2) \otimes SU(2)) \otimes SU(2)$ instead of $SO(4) \otimes SU(2)$. This is possible since the Lie algebras of thes two groups are the same, but the global groups are not isomorphic but homomorphic. Similarly, it is more accurate to say that the non-invariance group is $Sp(2,2) \otimes SU(2)$.

In the notation of Strom (18), it is the $\pi^{(+)}_{\frac{1}{2},\frac{1}{2}}$ representation of the 1 + 4 de Sitter group's Lie algebra which is realized in the present problem. The representations of this group, which is locally

isomorphic to $Sp(2,2)$ and $SO(4,1)$, were first classified by Dixmier (19). However, when he gave the matrix elements of the Lie algebra, he used the basis corresponding to the decomposition of the $SO(4)$ subgroup into the direct product of two $SU(2)$ groups. In other words, he used the representation space H given by the direct sum of representation spaces $H_{k,k'}$ for the $(2k + 1)(2k' + 1)$ dimensional representations of $SO(4)$:

$$H = \sum_{k,k'} \oplus H_{k,k'} \tag{46}$$

Ström (18) was the first to transform the basis to the basis corresponding to eigenfunctions of the J^2, J_z operators, which is the basis corresponding to the $\phi_{vk\mu}$ functions. Hence, we prefer to use his notation, since it enables a more direct comparison of the present problem with the representation theory.

In Ström's notation, the representations are classified into two classes, the continuous class of representations labeled $\nu_{r,\sigma}$ and the discrete class $\pi^{+}_{r,q}$, $\pi^{-}_{r,q}$, and $\pi_{r,0}$. The representations $\nu_{r,\sigma}$ are characterized by a parameter, σ, which can take on values in a semi-infinite interval, and by a discrete parameter r. Fradkin and Kiefer (20) showed that the $\nu_{\frac{1}{2},\sigma}$ representation is realized by the solutions of the Dirac Coulomb problem. The π type representations are characterized by the discrete parameters r and q, which satisfy the following restrictions:

i) for $\pi^{+}_{r,q}$ $r = \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$ and $q = r, r-1, 1, \ldots 1$ or $\frac{1}{2}$ where $r \geq n \geq q$, $r = \min(k + k')$

ii) for $\pi^{-}_{r,q}$ $r = \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$ and $q = r, r-1, \ldots 1$ or $\frac{1}{2}$ where $r \geq -n \geq q$, $r = \min(k + k')$

iii) for $\pi_{r,o}$, $r = 1,2,3,\ldots$ $q = 0$, $2k = 2k' \geq r$.

The Lie algebra of $SU(2,2)$ consists of 15 generators, whereas $Sp(2,2)$ and $SO(4,1)$ have 10 generators. We have already remarked that $Sp(2,2)$ and $SO(4,1)$ have the same Lie algebra, and that due to the actual values of (j_1, j_2) realized by the problem, it is better to call the invariance group as $Sp(2,2) \otimes SU(2)$. The group $SU(2,2)$ is the group of 4×4 complex matrices which leave invariant the form

$$|x_1|^2 + |x_2|^2 - |x_3|^2 - |x_4|^2 \tag{47}$$

If we also require invariance of the bilinear form

$$x_1 \xi_2 - x_2 \xi_1 + x_3 \xi_4 - x_4 \xi_3$$

we get the subgroup $Sp(2,2)$.

Again, the group $SU(2,2)$ has 15 generators, whereas $Sp(2,2)$ and $SO(4,1)$ have 10. The generators of $SU(2,2)$ were labeled by Yao (21) as $\vec{J}$, $\vec{K}$, P_+, P_-, Q_+, Q_-, S_+, S_-, T_+, T_-, R_o and the generators of $Sp(2,2)$ were

$$\vec{J}, \vec{K}, P_+ + Q_+, Q_+ + P_-, S_+ - T_-, T_+ - S_-. \tag{48}$$

To enlarge this to $SO(4,2)$ or $SU(2,2)$ one must add the operators

$$R_0, P_- - Q_+, Q_- - P_+, S_- + T_-, S_- + T_+ \tag{49}$$

By examining the matrix elements which Yao gives, it is possible to correspond his operators to the ones we have been using. We find:

$$\begin{aligned} P_+ + Q_- &\longrightarrow N_3 + T \\ P_- + Q_+ &\longrightarrow -N_3 + T \\ S_+ - T_- &\longrightarrow N_+ \\ -S_- + T_+ &\longrightarrow N_- \end{aligned} \tag{50}$$

By looking at these relations, it is possible to change some signs in the expressions for the operators $\vec{N}$ and T and come up with the extra operators of $SU(2,2)$. One can further check on this enlargement by studying the irreducible representations classified by Yao, and find that there is a representation of the E^- series which corresponds to the actual states realized in this problem. Hence, we have an $SU(2,2) \otimes SU(2)$ non-invariance group for the relativistic equivalent oscillator.

Although this Hamiltonian in spherical coordinates has been useful in some nuclear applications, it is, however, not suitable as a model for fission studies. The relativistic equivalent oscillator in cylindrical coordinates, which is really suited for this work, will form the content of the following chapter.

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CHAPTER III

A RELATIVISTIC EQUIVALENT OSCILLATOR IN CYLINDRICAL COORDINATES

Having discussed the invariance and non-invariance properties of the relativistic equivalent oscillator in spherical coordinates in the previous chapter, we now introduce a relativistic equivalent oscillator in cylindrical coordinates. After discussing the non-relativistic harmonic oscillator in cylindrical coordinates, we will examine the relativistic equivalent oscillator, and then the corresponding two center models. These latter two center models are useful in the calculation of shell corrections to fission barriers, as we shall see in later chapters.

The three dimensional, isotropic harmonic oscillator Hamiltonian:

$$H = \frac{1}{2m} p^2 + \frac{1}{2} m\omega^2 r^2 \tag{1}$$

leads in cylindrical coordinates (ρ, ϕ, z) to the equation

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\phi^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}m\omega^2(\rho^2+z^2)\right)\psi = 0 \tag{2}$$

which is of the separable type (see Fong (1)). The solutions are

$$\psi_{pmn_z}(\rho,\phi,z) = F_{p|m|}(\rho)\,\Phi_m(\rho)\,u_{n_z}(z) \tag{3}$$

where

$$F_{p|m|}(\rho) = \sqrt{\frac{2\lambda\,\Gamma(p+|m|+1)}{p!\,[\Gamma(|m|+1)]^2}}\; e^{-\frac{(\lambda\rho)^2}{2}} (\lambda\rho)^{|m|}\, {}_1F_1(-p, |m|+1; (\lambda\rho)^2) \tag{4}$$

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}}\, e^{im\phi} \tag{5}$$

$$u_{n_z}(z) = \frac{\lambda}{\sqrt{2^{n_z}\, n_z!\, \sqrt{\pi}}}\, e^{-\frac{(\lambda z)^2}{2}} H_{n_z}(\lambda z) \tag{6}$$

Here ${}_1F_1(a,c,x)$ is the confluent hypergeometric function and $H_{n_z}(\lambda z)$ is the Hermite polynomial of order n_z. The energy eigenvalue is given by

$$E = \frac{\lambda^2 (\hbar c)^2}{m_0 c^2}\left(2p + |m| + n_z + \frac{3}{2}\right) \tag{7}$$

where $$\lambda^2 = \frac{m_0 \omega}{\hbar}$$

and the quantum numbers p, m, n_z take on the values

$$p = 0, 1, 2, \ldots$$

$$m = 0, \pm 1, \pm 2, \ldots \tag{8}$$

$$n_z = 0, 1, 2, \ldots$$

In spherical coordinates, the solutions were

$$\psi_{v\ell m}(r, \theta, \phi) = F_{v\ell}(r)\, Y_\ell^m(\theta, \phi) \tag{9}$$

and there exists a transformation which gives the solutions in cylindrical coordinates as an expansion in terms of spherical coordinates solutions for the same energy and m value. We give the first few of these expansions in Table 1.

The relativistic equivalent oscillator Hamiltonian in cylindrical coordinates, which has been introduced by Swamy and Chaffin (2), is given by

$$H = \rho_1 \vec{\sigma}\cdot\vec{p} + \lambda^2[\rho_1(\vec{r}\times\vec{\sigma})_z + \rho_2 z] + \rho_3 m_0 \tag{10}$$

For $m > 0$ it has the solutions

$$\psi_1^{(+)} = \begin{bmatrix} -2\lambda i\sqrt{p+m+1}\, F_{pm}\phi_m u_{n_z} \\ -\sqrt{2}\lambda i\sqrt{n_z+1}\, F_{p\,m+1}\phi_{m+1}u_{n_z+1} \\ 0 \\ (E-m_0)F_{p,m+1}\phi_{m+1}u_{n_z} \end{bmatrix} \frac{1}{\sqrt{2E(E-m_0)}} \tag{11}$$

and

$$\psi_2^{(+)} = \begin{bmatrix} -\sqrt{2}\lambda i\sqrt{n_z+1}\, F_{pm}\phi_m u_{n_z} \\ 2\lambda i\sqrt{p+m+1}\, F_{p\,m+1}\phi_{m+1}u_{n_z+1} \\ (E-m_0)F_{p\,m}\phi_m u_{n_z+1} \\ 0 \end{bmatrix} \frac{1}{\sqrt{2E(E-m_0)}} \tag{12}$$

with energy eigenvalue

$$E = \sqrt{m_0^2 + 4\lambda^2(p+m+\tfrac{1}{2}n_z+3/2)} \tag{13}$$

TABLE I

SPHERICAL AND CYLINDRICAL COORDINATES
BASIS FUNCTIONS

Level	$\psi_{pmn_z}(\rho,\phi,z) = \sum_{v\ell} A^{v\ell m}_{pmn_z} F_{v\ell}(r) Y^m_\ell(\theta,\phi)$
n = 0	$\psi_{000}(\rho,\phi,z) = \sqrt{\frac{\lambda^3}{\pi^{3/2}}} e^{-(\lambda\rho)^2/2} e^{-(\lambda z)^2/2} \equiv F_{00}(r) Y^0_0(\theta,\phi)$
n = 1	$\psi_{001}(\rho,\phi,z) = \sqrt{\frac{2\lambda^3}{\pi^{3/2}}} (\lambda z) e^{-(\lambda\rho)^2/2} e^{-(\lambda z)^2} \equiv F_{01}(r) Y^0_1(\theta,\phi)$
	$\psi_{010}(\rho,\phi,z) = \sqrt{\frac{\lambda^3}{\pi^{3/2}}} (\lambda\rho) e^{-(\lambda\rho)^2/2} e^{i\phi} e^{-(\lambda z)^2} \equiv F_{01}(r) Y^1_1(\theta,\phi)$
	$\psi_{0-10}(\rho,\phi,z) = \sqrt{\frac{\lambda^3}{\pi^{3/2}}} (\lambda\rho) e^{-(\lambda\rho)^2} e^{-i\phi} e^{-(\lambda z)^2} \equiv F_{01}(r) Y^{-1}_1(\theta,\phi)$
n = 2	$\psi_{100}(\rho,\phi,z) = \sqrt{\frac{\lambda^3}{\pi^{3/2}}} (1-(\lambda\rho)^2) e^{-(\lambda\rho)^2} e^{-(\lambda z)^2} \equiv \sqrt{\frac{2}{3}} F_{10} Y^0_0 + \sqrt{\frac{1}{3}} F_{02} Y^0_2$
	$\psi_{020}(\rho,\phi,z) = \sqrt{\frac{\lambda^3}{2\pi^{3/2}}} (\lambda\rho) e^{-(\lambda\rho)^2} e^{i2\phi} e^{-(\lambda z)^2} \equiv F_{02}(r) Y^2_2(\theta,\phi)$
	$\psi_{0-20}(\rho,\phi,z) = \sqrt{\frac{\lambda^3}{2\pi^{3/2}}} (\lambda\rho) e^{-(\lambda\rho)^2} e^{-i2\phi} e^{-(\lambda z)^2} \equiv F_{02}(r) Y^{-2}_2(\theta,\phi)$
	$\psi_{002}(\rho,\phi,z) = \sqrt{\frac{2\lambda^3}{\pi^{3/2}}} e^{-(\lambda\rho)^2} \left[(\lambda z)^2 - \frac{1}{2}\right] e^{-(\lambda z)^2} \equiv -\sqrt{\frac{1}{3}} F_{10} Y^0_0 + \sqrt{\frac{2}{3}} F_{02} Y^0_2$
	$\psi_{011}(\rho,\phi,z) = \sqrt{\frac{2\lambda^3}{\pi^{3/2}}} e^{-(\lambda\rho)^2} (\lambda\rho) e^{i\phi} (\lambda z) e^{-(\lambda z)^2} \equiv -F_{02}(r) Y^1_2(\theta,\phi)$
	$\psi_{0-11}(\rho,\phi,z) = \sqrt{\frac{2\lambda^3}{\pi^{3/2}}} e^{-(\lambda\rho)^2} (\lambda\rho) e^{-i\phi} (\lambda z) e^{-(\lambda z)^2} \equiv F_{02}(r) Y^{-1}_2(\theta,\phi)$

For fixed values of p, m, n_z, the above two solutions are linearly independent. However, there exist two more forms which are not linearly independent of the above, but which are nevertheless useful. They are given by

$$\psi_3^{(+)} = \begin{bmatrix} 0 \\ (E+m_0) F_{p,m+1} \phi_{m+1} u_{n_z+1} \\ -2\lambda i \sqrt{p+m+1}\, F_{pm} \phi_m u_{n_z+1} \\ \sqrt{2}\lambda i \sqrt{n_z+1}\, F_{p\,m+1} \phi_{m+1} u_{n_z} \end{bmatrix} \frac{1}{\sqrt{2E(E+m_0)}} \tag{14}$$

and

$$\psi_4^{(+)} = \begin{bmatrix} (E+m_0) F_{pm} \phi_m u_{n_z} \\ 0 \\ \sqrt{2}\, i\lambda \sqrt{n_z+1}\, F_{pm} \phi_m u_{n_z+1} \\ 2i\lambda \sqrt{p+m+1}\, F_{p\,m+1} \phi_{m+1} u_{n_z} \end{bmatrix} \frac{1}{\sqrt{2E(E+m_0)}} \tag{15}$$

For $m < 0$ the four forms are

$$\psi_1^{(-)} = \begin{bmatrix} 2i\lambda \sqrt{p+1}\, F_{p|m|} \phi_m u_{n_z} \\ -\sqrt{2}\, i\lambda \sqrt{n_z+1}\, F_{p+1,|m|-1} \phi_{m+1} u_{n_z+1} \\ 0 \\ (E-m_0) F_{p+1,|m|-1} \phi_{m+1} u_{n_z} \end{bmatrix} \frac{1}{\sqrt{2E(E-m_0)}} \tag{16}$$

$$\psi_2^{(-)} = \begin{bmatrix} -\sqrt{2}\, i\lambda \sqrt{n_z+1}\, F_{p|m|} \phi_m u_{n_z} \\ -2i\lambda \sqrt{p+1}\, F_{p+1,|m|-1} \phi_{m+1} u_{n_z+1} \\ (E-m_0) F_{p|m|} \phi_m u_{n_z+1} \\ 0 \end{bmatrix} \frac{1}{\sqrt{2E(E-m_0)}} \tag{17}$$

$$\psi_3^{(-)} = \begin{bmatrix} 0 \\ (E+m_0)\, F_{p+1,|m|-1}\, \phi_{m+1}\, u_{n_z+1} \\ 2i\lambda\sqrt{p+1}\, F_{p|m|}\, \phi_m\, u_{n_z+1} \\ \sqrt{2}\, i\lambda\sqrt{n_z+1}\, F_{p+1,|m|-1}\, \phi_{m+1}\, u_{n_z} \end{bmatrix} \frac{1}{\sqrt{2E(E+m_0)}} \tag{18}$$

$$\psi_4^{(-)} = \begin{bmatrix} (E+m_0)\, F_{p|m|}\, \phi_m\, u_{n_z} \\ 0 \\ \sqrt{2}\, i\lambda\sqrt{n_z+1}\, F_{p|m|}\, \phi_m\, u_{n_z+1} \\ -2i\lambda\sqrt{p+1}\, F_{p+1,|m|-1}\, \phi_{m-1}\, u_{n_z} \end{bmatrix} \frac{1}{\sqrt{2E(E+m_0)}} \tag{19}$$

For all four solutions the energy eigenvalue is given by

$$E = \sqrt{m_0^2 + 4\lambda^2\left(p + \tfrac{1}{2}n_z + \tfrac{3}{2}\right)} \tag{20}$$

The validity of the above solutions may be demonstrated by using the following ladder relations:

$$\left[\frac{d}{d\rho} + \frac{\mu}{\rho} + \lambda^2\rho\right] F_{p\mu} = 2\lambda\sqrt{p+\mu}\, F_{p,\mu-1} \qquad \mu = |m| \tag{21}$$

$$\left[\frac{d}{d\rho} + \lambda^2\rho\right] F_{p0} = -2\lambda\sqrt{p}\, F_{p-1,1} \tag{22}$$

$$\left[\frac{d}{d\rho} - \frac{\mu}{\rho} - \lambda^2\rho\right] F_{p\mu} = -2\lambda\sqrt{p+\mu+1}\, F_{p,\mu+1} \tag{23}$$

$$\left[\frac{d}{d\rho} - \lambda^2\rho\right] F_{p0} = -2\lambda\sqrt{p+1}\, F_{p1} \tag{24}$$

$$\left[\frac{d}{d\rho} - \frac{\mu}{\rho} + \lambda^2\rho\right] F_{p\mu} = -2\lambda\sqrt{p}\, F_{p-1,\mu+1} \tag{25}$$

$$\left[\frac{d}{d\rho} + \frac{\mu}{\rho} - \lambda^2\rho\right] F_{p\mu} = 2\lambda\sqrt{p+1}\, F_{p+1,\mu-1} \tag{26}$$

$$\left(\frac{d}{dz} + \lambda^2 z\right) u_{n_z} = \sqrt{2}\lambda\sqrt{n_z}\, u_{n_z-1} \tag{27}$$

$$\left(\frac{d}{dz} - \lambda^2 z\right) u_{n_z} = -\sqrt{2}\lambda\sqrt{n_z+1}\, u_{n_z+1} \tag{28}$$

Having introduced the above relativistic equivalent oscillator in cylindrical coordinates, the next formal step would be to consider the form of the potential and proceed to classify it according to transformation properties under the Lorentz group. We find that we can write equation (10) in the form

$$\left\{\gamma^\mu\left(\frac{\partial}{\partial x^\mu} - iA_\mu\right) + m_0 - i\gamma_5 U_{ps}\right\}\psi = 0 \tag{29}$$

where

$$A_0 = 0 \qquad U_{ps} = \lambda^2 z$$
$$A_1 = \lambda^2 y \qquad \vec{\gamma} = -i\beta\vec{\gamma}$$
$$A_2 = -\lambda^2 z \qquad \gamma_4 = \beta \tag{30}$$
$$A_3 = 0 \qquad \gamma_5 = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

Thus, we apparently have a vector potential A_μ plus a pseudoscalar potential U_{ps}. However, problems arise when we consider the restrictions which the commutation of parity and total angular momentum place upon these potentials (see Miller, reference (3)). These restrictions are found to be that the pseudoscalar type potentials must vanish, and

the vector type potentials have to be of the form

$$U_r^0(\vec{r}) = 0$$
$$\vec{U}_v^r(\vec{r}) = \hat{r}\, U_v(r) \tag{31}$$

The potentials we have here obviously violate this and it is not surprising that we find that $\vec{J}$ does not commute with them.

If a Hamiltonian used to describe a problem possessing spherical symmetry violates this symmetry, a modification of this can at times be made to conform to spherical symmetry. Briefly, what we propose to do is to: 1) Perform a Foldy-Wouthuysen transformation on the Hamiltonian of equation (10), 2) Identify any terms which violate spherical symmetry, and 3) Add the negative of such terms to the Dirac Hamiltonian of equation (10). Such a procedure will be valid only in cases where a Foldy-Wouthuysen type expansion is valid. This will be the case in nuclei, since it is known that relativistic corrections are but a few per cent. We will discuss this procedure in detail in a later chapter.

We have already remarked that the angular momentum operators do not commute with equation (10). Hence, we might expect an unusual type of invariance group to be present. By inspecting the energy eigenvalue of equation (20), valid for $m < 0$, we see that this eigenvalue is independent of m. Hence the degeneracy of the energy levels will be infinite. There is a theorem in group theory which states that irreducible unitary representations of a group are finite if and only if the group is compact (see Fronsdal (4)). Hence, unless this is an exception to the theorem, we should expect the invariance group to be non-compact, hence it cannot be SU(3), SO(4), etc.

The solutions to two center oscillator Hamiltonian in one dimension were first given by Merzbacher in the first edition of his Quantum Mechanics (5). The solutions for the three dimensional problem were given by references (6) and (7). This two center oscillator Hamiltonian is given by

$$H = \frac{1}{2m}p^2 + \frac{1}{2}\frac{\lambda^4(\hbar c)^2}{m_0 c^2}\begin{cases}(z+z_0)^2+\rho^2 & z \le 0\\ (z-z_0)^2+\rho^2 & z \ge 0\end{cases} \tag{31}$$

For $z_0 = 0$ it reduces to equation (1), while for $z_0 \neq 0$ the potential is that of two harmonic oscillator wells separated by $2z_0$ and joined in a cusp. The problem is still of the separable type, and remarkably enough, it still possesses exact solutions. Only the z part of the solution changes, and this solution is given by

$$U_{n_z}(z) = \begin{cases} N^{n_z} D_{n_z}\left(\sqrt{2}\lambda(z-z_0)\right) & z \ge 0\\ \pm N^{n_z} D_{n_z}\left(-\sqrt{2}\lambda(z+z_0)\right) & z \le 0\end{cases} \tag{32}$$

Here $D_{n_z}(x)$ is Weber's parabolic cylinder function, given by

$$D_{n_z}(x) = 2^{n_z/2} e^{-x^2/4}\left[\frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1-n_z}{2})}\,{}_1F_1\left(-\tfrac{1}{2}n_z, \tfrac{1}{2}; \tfrac{1}{2}x^2\right)\right.$$

$$\left. + \frac{x}{\sqrt{2}}\frac{\Gamma(-\frac{1}{2})}{\Gamma(-\frac{1}{2}n_z)}\,{}_1F_1\left(\frac{1-n_z}{2}, \frac{3}{2}; \tfrac{1}{2}x^2\right)\right] \tag{33}$$

When $z_0 \neq 0$, n_z is a non-integral quantum number determined by requiring $U_{n_z}(z)$ and its first derivative to be continuous at $z = 0$. This leads to the conditions

$$D_{n_z}(-\sqrt{2}\lambda z_0) = 0 \qquad \text{(odd parity)} \qquad (34)$$

$$D'_{n_z}(-\sqrt{2}\lambda z_0) = 0 \qquad \text{(even parity)} \qquad (35)$$

Having given the solutions to the above non-relativistic problem, we would now like to introduce the two-center relativistic equivalent oscillator in cylindrical coordinates. This Hamiltonian is:

$$H_{①} = \begin{cases} \rho_1 \sigma\cdot p + \lambda^2\left[\rho_1(\vec{r}\times\vec{\sigma})_z + \rho_2(z-z_0)\right] + \rho_3 m_0 & z \geq 0 \\ \rho_1 \sigma\cdot p + \lambda^2\left[\rho_1(\vec{r}\times\vec{\sigma})_z + \rho_2(z+z_0)\right] + \rho_3 m_0 & z \leq 0 \end{cases} \qquad (36)$$

A typical solution is given by the same formulas as equations (11)-(19), with $u_{n_z}(z)$ replaced by the $U_{n_z}(z)$ of equation (32), and n_z by the corresponding quantum number.

However, this gives a solution only when $U_{n_z}(z)$ has odd parity (unless $z_0 = 0$). To get an even function of z in the upper component, we must use U_{n_z-1}. For instance, equation (11) must be written as

$$\psi_1^{(4)} = \frac{1}{\sqrt{2E(E-m_0)}} \begin{bmatrix} -2\lambda i\sqrt{p+m+1}\, F_{pm}\phi_m U_{n_z-1} \\ -\sqrt{2}\lambda i\sqrt{n_z+1}\, F_{p\,m+1}\phi_{m+1} U_{n_z} \\ 0 \\ (E-m_0) F_{p,m+1}\phi_{m+1} U_{n_z-1} \end{bmatrix} \qquad (37)$$

The reason for the above difference between odd parity and even parity cases is related to the discontinuity of the potential of equation (36) at $z = 0$.

For the case of the one dimensional Schrödinger equation, one knows that

$$\frac{d\psi}{dx}(x_0+\epsilon) - \frac{d\psi}{dx}(x_0-\epsilon) = \int_{x_0-\epsilon}^{x_0+\epsilon} \frac{2\mu}{\hbar^2}\left[V(x)-E\right]\psi(x)\,dx \tag{38}$$

For reasonably well behaved potentials, including the potential of equation (31), the integral on the right of this equation is zero. Hence, the derivative of the wavefunction must be continuous.

For the case of the above Dirac equation

$$\frac{d\psi}{dz}(0+\epsilon) - \frac{d\psi}{dz}(0-\epsilon) = -2\lambda^2 z_0 \rho_3 \psi(z=0) \tag{39}$$

We obtain this since the derivative of the step function

$$f(z) = \begin{cases} z_0 & z \leq 0 \\ -z_0 & z \geq 0 \end{cases} \tag{40}$$

gives the Dirac delta function:

$$\frac{d}{dz} f(z) = -2z_0\,\delta(z) \tag{41}$$

For the case where $U_{n_z}(z)$ is zero at $z = 0$, i.e. for non-relativistic solutions of odd parity, the right hand side of equation (39) is zero. Hence, components containing these odd functions of z (for which $D_{n_z}(-\sqrt{2}\lambda z_0) = 0$) will be continuous and have continuous derivatives. However, where even functions of z which are not zero at $z = 0$ are

involved, the Dirac equation requires a discontinuity of the derivative at $z = 0$.

Care is needed in constructing the relativistic solutions, in order to avoid a discontinuous wavefunction. The Dirac equation requires the wavefunction to be continuous; it is only the derivative which may possibly be discontinuous in a given component. This is the reason for the statement made earlier, that, to get an even function of z in the upper component, one must use $U_{n_z-1}(z)$. If one tried to use $U_{n_z}(z)$, where n_z was a solution of equation (35), then the function $U_{n_z+1}(z)$ occuring in the second component would be discontinuous at $z = 0$, and hence, we would get a wrong wavefunction.

A question arises, however, at this point, whether a discontinuity of the derivative of the wavefunction might not be inconsistent with its physical interpretation. In the case of the Schrödinger equation, one knows the probability current density to be

$$\vec{j} = \frac{\hbar}{2m}\left(\psi^* \frac{\hbar}{i}\nabla\psi - \psi\frac{\hbar}{i}\nabla\psi^*\right)$$
$$\rho = \psi^*\psi \tag{42}$$

In that case, the discontinuity of the wavefunction would imply a discontinuity in the probability current density, and the continuity equation

$$\nabla\cdot\vec{j} + \frac{\partial\rho}{\partial t} = 0 \tag{43}$$

would be violated. However, for the Dirac equation the current density is given by

$$\vec{j} = c\psi^* \vec{\nabla} \psi \qquad (44)$$

$$\rho = \psi^* \psi$$

so that $\vec{j}$ is not proportional to the derivative of ψ and the physical interpretation is consistent.

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CHAPTER IV

SHELL CORRECTIONS IN FISSION THEORY

The liquid drop model of nuclear fission, introduced by Bohr and Wheeler (1) and by Frenkel (2) is known to provide a satisfactory description of the process at high excitation energies, when fluctuation effects associated with the presence of shell structure in the nuclei can be neglected.

The semi-empirical mass formula contains three terms which come from the liquid drop model. The first is the volume energy, i.e. the average energy due to bonds between nucleons.This term gives the nucleus the right density but does not control its extent. The second and third terms are the Coulomb energy of the uniformly charged droplet, and the surface energy. The surface energy is the decrease in binding energy due to the presence of unsaturated bonds formed by nucleons at the surface. When we consider deformations of the nucleus which occur during fission, one usually considers that the volume energy does not depend on the nuclear shape, i.e. nuclear matter is incompressible. Thus, the Coulomb and surface energies are responsible for the change in energy of the charged drop at various deformations, that is, they define the potential energy surface. At high excitation energies, these terms give a satisfactory description of the fission process.

For low excitation energies, theoretical studies have shown that single particle effects can be employed very successfully in the

explanation of the failures of the liquid drop model. It was known for some time that these single particle effects could be qualitatively connected with the observed characteristics of mass and energy distributions. However, before the work of Strutinsky (3), it was not clear how to quantitatively calculate the change in potential energy due to these single particle effects. Consequently, it was even more uncertain as to what these shell effects would do to inertial parameters and the dynamics of the fission process.

In this chapter, we discuss the shell corrections, and in particular the various models based upon the two center oscillator Hamiltonian. This two center model remains applicable for large separations of the two centers, i.e. for large deformations and then even for the asymptotic limit of two fragments separated to infinity. It is advantageous to consider relativistic extensions of the two-center models, since we would like to find out if relativistic corrections become larger at large deformations.

In Strutinsky's method, one calculates the shell corrections for an N-particle nucleus via the equation:

$$\Delta E_{SC}(N) = \sum_{n=1}^{N} \epsilon_n - \int_0^N \bar{\epsilon}(n)\,dn \qquad (1)$$

Here, the summation is over the single particle energies of the filled levels of the shell model, and the integration is over a smooth function $\bar{\epsilon}(n)$ that specified the average behaviour of the single particle energy as a function of particle number n. In the method of evaluation discussed by Bolsterli, et al. (4), we find this smooth function by

expanding the Dirac delta function in a series of Hermite polynomials, and retaining the first five or six terms only. Thus, we have:

$$\frac{1}{\gamma}\sum_{n=1}^{\infty}\delta(u_n) = \frac{1}{\gamma\sqrt{\pi}}\sum_{n=1}^{\infty} e^{-u_n^2}\sum_{m=0}^{\infty} c_m H_m(u_n) \tag{2}$$

where

$$c_m = \begin{cases} \dfrac{(-1)^{m/2}}{2^m\left(\frac{m}{2}\right)!}, & m \text{ even} \\ 0, & m \text{ odd} \end{cases} \tag{3}$$

and

$$u_n = \frac{\epsilon - \epsilon_n}{\gamma} \tag{4}$$

If we retain only the first six terms in the sum over m, we get the smooth level density, and the result

$$\int_0^N \bar{\epsilon}(n)\,dn = \sum_{n=1}^{\infty}\left\{\frac{1}{2}\epsilon_n\left[1+\operatorname{erf}(\bar{u}_n)\right] - \frac{1}{2\sqrt{\pi}}\gamma e^{-u_n^2} - \frac{1}{\sqrt{\pi}}e^{-u_n^2}\sum_{m=1}^{6} c_m\left[\frac{1}{2}\gamma H_m(\bar{u}_n) + \epsilon_n H_{m-1}(\bar{u}_n) + m\gamma H_{m-2}(\bar{u}_n)\right]\right\} \tag{5}$$

Here

$$\bar{u}_n = \frac{\bar{\lambda} - \epsilon_n}{\gamma} \tag{6}$$

where $\bar{\lambda}$ is the Fermi energy.

In Figure 1 we show a plot of the potential energy in MeV as a function of deformation for the nucleus ^{240}Pu. The smooth trend of

this curve is obtained from the liquid drop model. The small wiggles near zero deformation are obtained using the shell and pairing corrections of Strutinsky (4). The ^{240}Pu nucleus is deformed in the ground state, as we can see from the minimum in the curve just to the right of the zero deformation line. The second minimum to the right of the zero deformation line is predicted by the shell correction theory, and its existence is experimentally confirmed via shape isomers, the energy dependence of the cross section for induced fission (see Figure 2), and by the angular distribution of Fission fragments as interpreted in terms of Aage Bohr's channel theory of fission (6).

In Figure 3 we show two hypothetical plots of energy levels of bound nuclei. The arrows point out the Fermi level. In the case shown on the left the density of levels is small near the Fermi level, while in the other case it is large. The former case will correspond to a decrease in the potential energy caused by the small level density, i.e. the nucleus with the level scheme shown on the left will be "more bound" than the one on the right.

Before Strutinsky introduced his shell correction, it seemed to be undisputed that any quantum shell effect decreased with increasing deformation and therefore could not play any significant role at the large deformations which take place in the fission process. However, Strutinsky introduced the definition of a magic nucleus as being one which has the lowest density (among its neighbors) of levels near the Fermi level. When one uses this definition to study shell effects, it

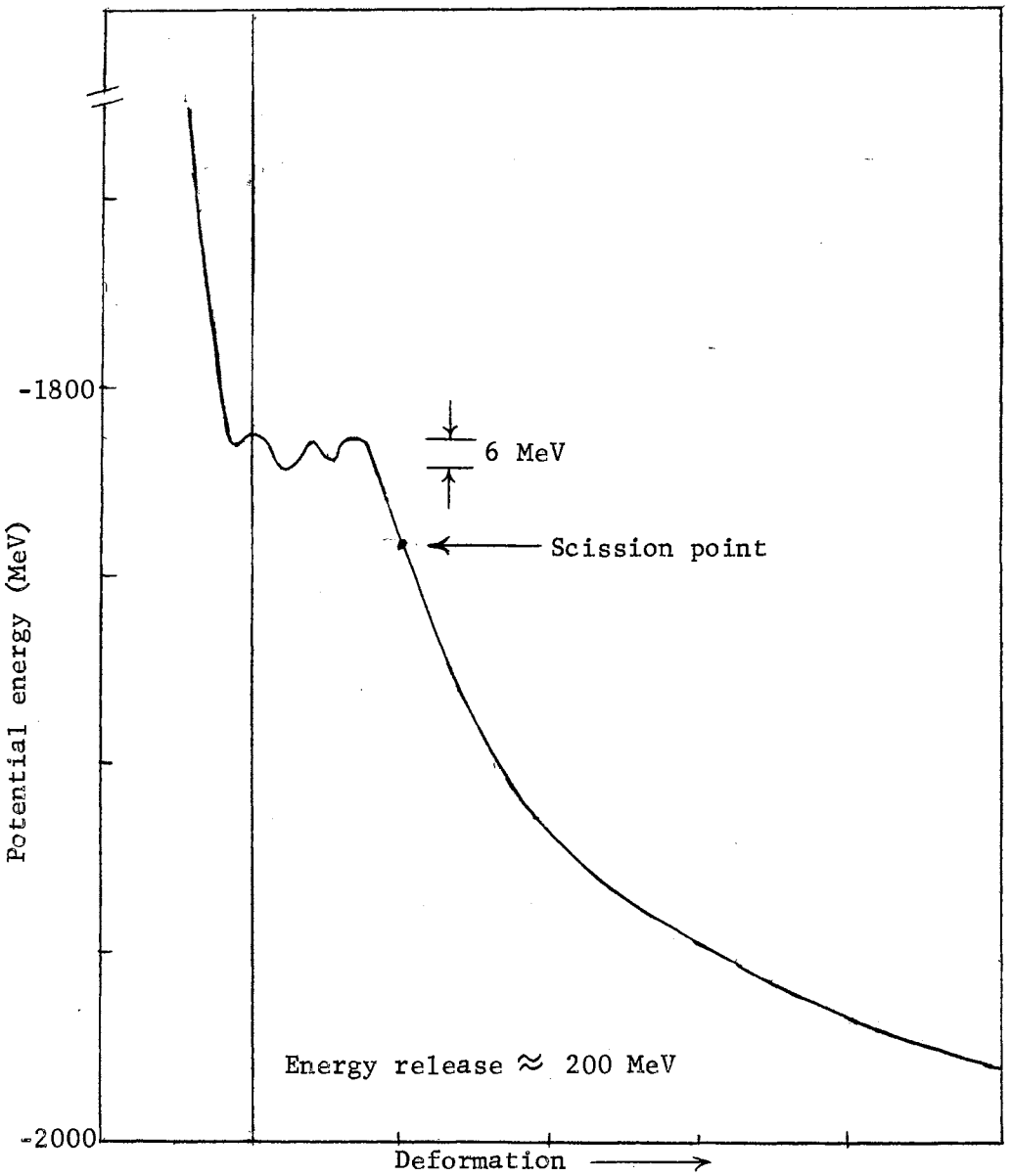

Figure 1. Plot of Potential Energy in MeV Versus Deformation for ^{240}Pu (After Bolsterli, et al. (1972)).

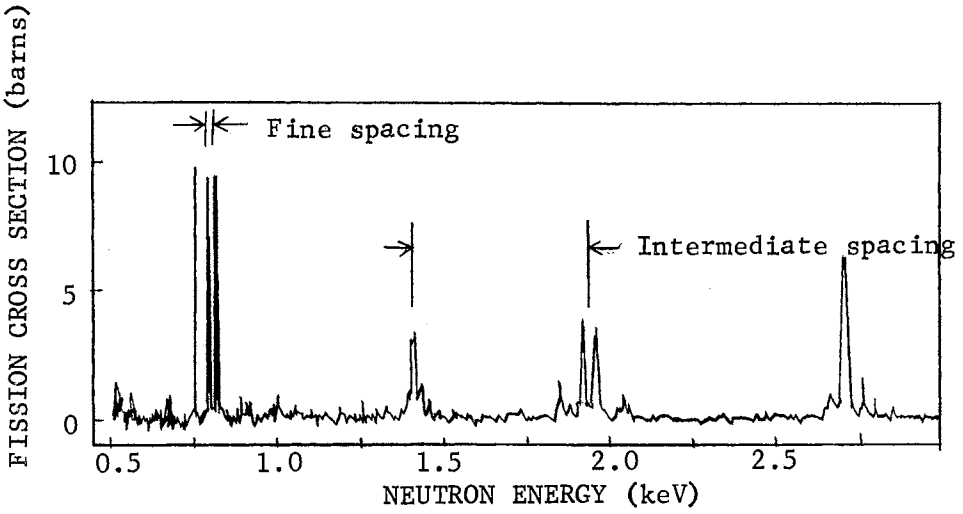

Figure 2. Cross-section Resonance Structure in Subbarrier (n,f) Reactions Was Hard to Understand before the Double Humped Barrier Was Postulated. The intermediate structure of the ^{240}Pu reaction is now well correlated with the energy level density in the second well. (After Clark, Ref. (5)).

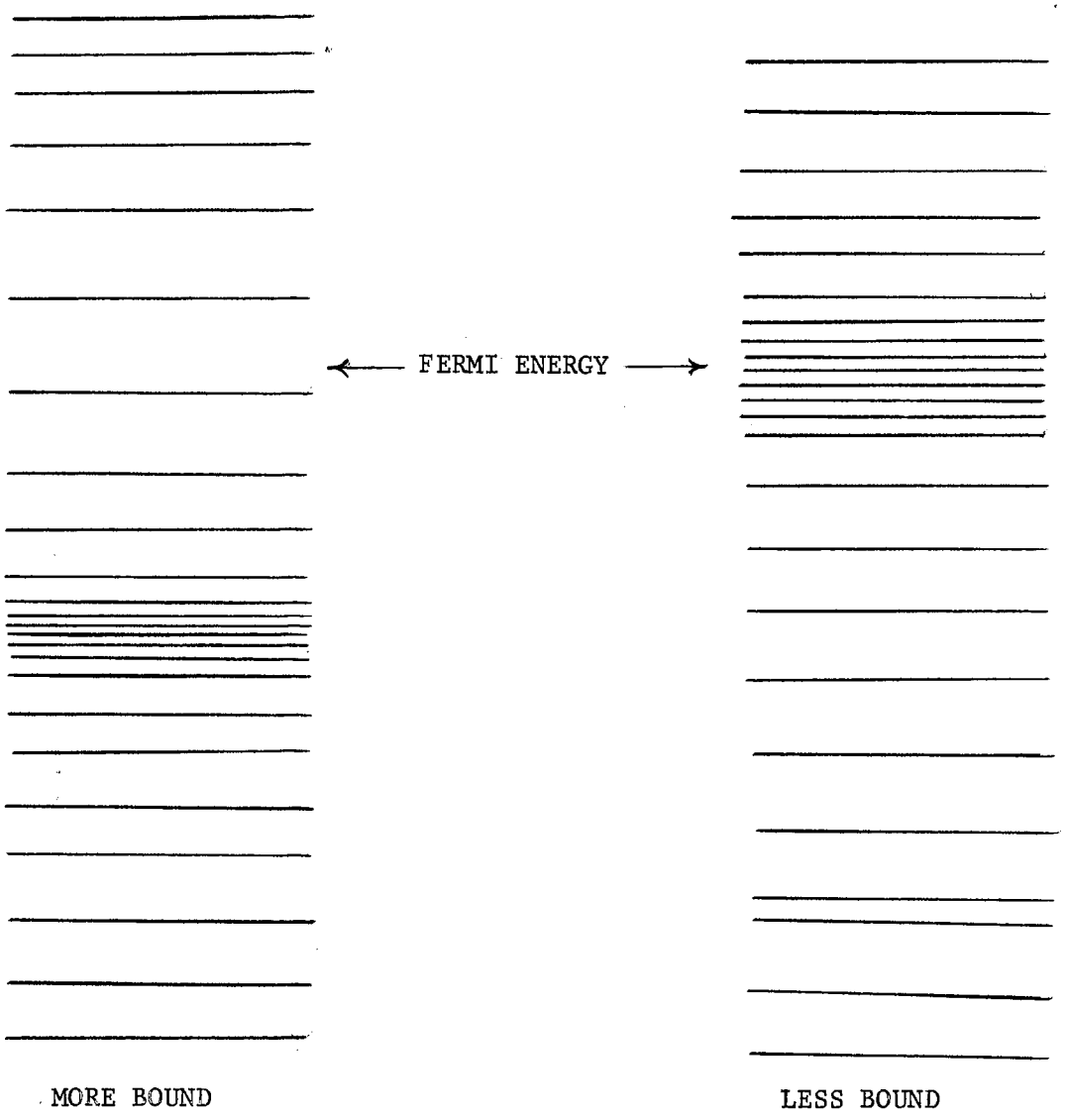

Figure 3. Single Particle Energy Levels in a Bound Nucleus

becomes evident that shell effects do not vanish in deformed nuclei. This is illustrated in Figure 4, a plot of some hypothetical energy levels versus deformation. The illustration has circles in it showing regions of low level density. It is evident that nuclei with Fermi levels in these regions will be more bound than otherwise.

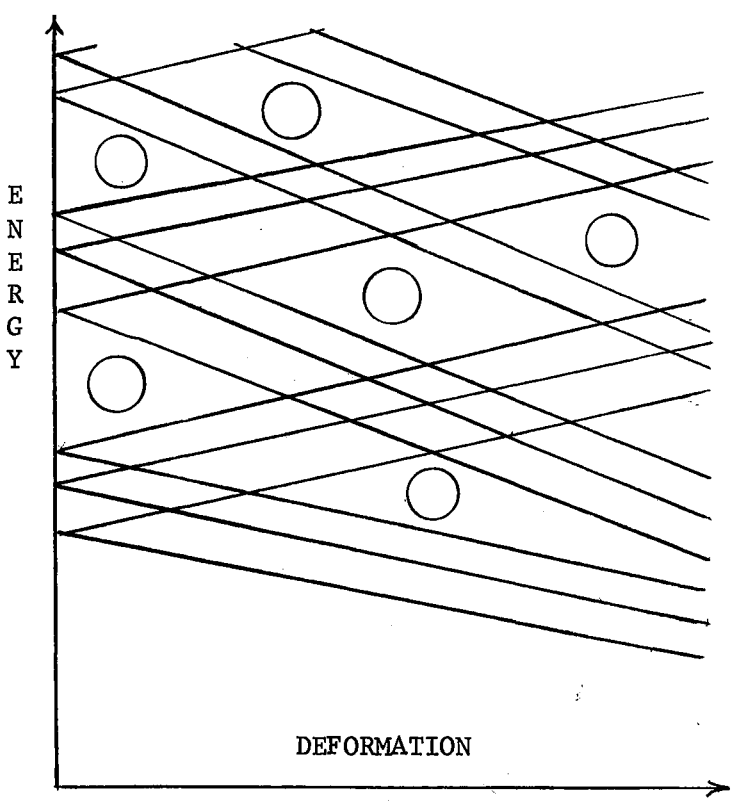

Figure 4. A Hypothetical Level Scheme Showing Regions with Low Level Density with Circles.

From the above discussion, we see that in order to estimate shell corrections to the potential energy surface, one needs a model which

gives energy levels as a function of deformation. The various models include parametrizations based upon Woods Saxon wells, one center oscillator wells, and two center oscillator wells. We will restrict our discussion to the oscillator models.

The original one center oscillator model for deformed nuclei was given by S. G. Nilsson (7). In this model one starts with the Hamiltonian:

$$H = H_0 + C\,\ell\cdot s + D\ell^2 \tag{7}$$

where

$$H_0 = -\frac{\hbar^2}{2m}\Delta' + \frac{1}{2}M\left(\omega_x^2 x'^2 + \omega_y^2 y'^2 + \omega_z^2 z'^2\right)$$

For $\omega_x = \omega_y \neq \omega_z$, we have axially symmetric deformations of the type considered by B. Nilsson (8). In this case one may write the potential, including a term proportional to $P_4(\cos\theta)$ as

$$V = \frac{1}{2}\hbar\omega(\epsilon,\epsilon_4)\rho^2\left[1 - \frac{2}{3}\epsilon P_2(\hat{\xi},\hat{\eta},\hat{\zeta}) + 2\epsilon_4 P_4(\hat{\xi},\hat{\eta},\hat{\zeta})\right]$$
$$-\hbar\omega_0\kappa\left[2\,\ell\cdot s + \mu\left(\ell^2 - \langle\ell^2\rangle_{shell}\right)\right] \tag{8}$$

where ξ, η, ζ are the "stretched" coordinates:

$$\xi = x\sqrt{\frac{M\omega_\perp}{\hbar}} = \lambda_\perp x$$
$$\eta = y\sqrt{\frac{M\omega_\perp}{\hbar}} = \lambda_\perp y \tag{9}$$
$$\zeta = z\sqrt{\frac{M\omega_z}{\hbar}} = \lambda_z z$$

and we have added a term

$$-D\langle \ell^2 \rangle_{shell} = -D \tfrac{1}{2} N(N+3) \tag{10}$$

which keeps the ℓ^2 term from reducing the shell spacing (the separation between the average energies of shells N and $N+1$).

In this model, one determines the oscillator constant ω as a function of the deformation parameters ϵ and ϵ_4 by imposing the condition of constant volume. That is, since nuclear matter has a low compressibility and since nuclear forces have short range, we can determine ω by requiring the volume enclosed by the equipotential surfaces to be conserved. For example, for $\epsilon_4 = 0$ this leads to the equation

$$\omega_0 = \frac{\mathring{\omega}_0}{1 - \frac{1}{2}\epsilon^2 - \frac{2}{27}\epsilon^3} \tag{11}$$

In order to find the energy levels of a nucleus as a function of the above ϵ and ϵ_4 deformation parameters, one must diagonalize the matrix of the Hamiltonian starting from the basis for the isotropic harmonic oscillator. The application of the results of such a calculation to shell corrections has been reported by Nilsson et al. (9).

The two center oscillator Hamiltonian

$$H_0 = \frac{1}{2m} p^2 + \frac{1}{2} \frac{\lambda^4 (\hbar c)^2}{m_0 c^2} \begin{cases} (z+z_0)^2 + \rho^2 & z \leq 0 \\ (z-z_0)^2 + \rho^2 & z \geq 0 \end{cases} \tag{12}$$

has exact solutions for all values of z_0, as was discussed in Chapter 3. It has been introduced as a model for obtaining shell corrections by Greiner et al. (10-14). One simply copies the $\vec{l}\cdot\vec{s}$ and $\vec{l}^2$ terms of Nilsson and obtains

$$H = H_0 - \hbar\omega_0(z_0)\kappa \begin{cases} 2\vec{l}_1\cdot\vec{s} + \mu(\vec{l}_1^{\,2} - \frac{1}{2}N(N+3)) & z_0 \le 0 \\ 2\vec{l}_2\cdot\vec{s} + \mu(\vec{l}_2^{\,2} - \frac{1}{2}N(N+3)) & z_0 \ge 0 \end{cases} \tag{13}$$

Here $\vec{l}_1$ and $\vec{l}_2$ describe the angular momenta with respect to the two centers at $z = -z_0$ and $z = z_0$ respectively. We add these extra terms in order to obtain the correct energy level schemes at $z_0 = 0$ and $z_0 = \infty$, that is to match the known spins and parities of nuclei.

As in the Nilsson model, one determines ω (or λ) by the condition of constant volume. However, in this model, contrary to the Nilsson model, the conservation of the volume of any one equipotential does not lead to the same ω as another equipotential. Several prescriptions have therefore been tried, including conservation of the volume enclosed by the equipotential at the nuclear surface. However, in spite of the uncertainties in ω arising from this source, it has been found that calculated energy levels are rather insensitive to the choice of ω, as far as relative position is concerned.

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CHAPTER V

THE MODEL BASED ON THE DIRAC EQUATION

In Chapter III we introduced a relativistic equivalent oscillator in cylindrical coordinates, and extended it to a two center model. We mentioned the fact that for $z_0 = 0$ the Hamiltonian did not possess spherical symmetry, and suggested a procedure to correct this. This procedure, which makes use of the Foldy-Wouthuysen transformation, will be discussed in this chapter, and the details of the model for calculating the energy levels of the deformed nucleus will be discussed.

When one applies the Foldy Wouthuysen transformation to the Hamiltonian

$$H = \rho_1 \sigma \cdot p + \rho_3 m_0 + \lambda^2 \left[\rho_1 (\vec{r} \times \vec{\sigma})_z + \rho_2 z\right] \tag{1}$$

one gets, correct to order $1/m_0$

$$H_{FW} = \rho_3 m_0 + \frac{1}{2m_0}\rho_3 (p^2 + \lambda^4 r^2) + \rho_3 \frac{\lambda^2}{m_0}\left[L_z + \tfrac{1}{2}\sigma_z + \tfrac{1}{2}(1+\rho_3)\sigma_z\right] \tag{2}$$

We notice that, in addition to the rest mass and isotropic harmonic oscillator terms, we have additional terms which cause splittings between states with different m values. For states belonging to the same j, ℓ values, this splitting is a violation of spherical symmetry, and should not occur at $z_0 = 0$.

In order to remedy this situation, the following prescription is proposed. In the first step, we write down the new Dirac equation

$$H = \rho_1 \vec{\sigma}\cdot\vec{p}c + \lambda^2(\hbar c)\left[\rho_1(\vec{r}\times\vec{\sigma})_z + \rho_2 z\right] + \rho_3 m_0 c^2 - \rho_3 \frac{\lambda^2(\hbar c)^2}{m_0 c}\left[L_z + \frac{1}{2}\sigma_z + \sigma_z\right] \quad (3)$$

With the new term included, the Foldy-Wouthuysen transformation to order $1/m_0$ gives

$$H_{FW} = \rho_3 m_0 c^2 + \rho_3 \frac{1}{2m_0}(p^2 + \lambda^4\hbar^2 r^2) + \frac{1-\rho_3}{2}\frac{\lambda^2(\hbar c)^2}{m_0 c^2}\hbar\sigma_z \quad (4)$$

For positive energy states, we put $\rho_3 = 1$, and in this non-relativistic limit the spherical symmetry is restored. However, in higher order, there still exist terms violating spherical symmetry, and these must also be removed if we are to calculate the relativistic corrections properly. When we do the Foldy-Wouthuysen transformation to order $1/m_0^3$, we obtain

$$\begin{aligned} H_{FW} = {} & \rho_3 m_0 c^2 + \rho_3 \frac{1}{2m_0}(p^2 + \lambda^4 r^2) + \frac{1-\rho_3}{2}\frac{\lambda^2(\hbar c)^2}{m_0 c^2}\hbar\sigma_z \\ & + \frac{\lambda^4(\hbar c)^4}{2m_0^3 c^6}\rho_3 (L_z + \tfrac{1}{2}\sigma_z)^2 - \frac{\lambda^2(\hbar c)^2}{4m_0^3 c^6}(1+\rho_3)\hbar\sigma_z(p^2c^2 + \lambda^4(\hbar c)^2 r^2) \\ & - \frac{1}{8m_0^3 c^6}\rho_3(p^2c^2 + \lambda^4(\hbar c)^2 r^2)^2 - \frac{\lambda^4(\hbar c)^4}{4m_0^3 c^6}(\rho_3+1)\hbar^2 \\ & - \hbar\frac{\lambda^2(\hbar c)^2}{4m_0^3 c^5}\rho_3\left[\Omega_0, \rho_1 p_z c + \rho_2 \sigma_z z\right]_+ \end{aligned} \quad (5)$$

We will discuss the removal of the contributions of the objectionable terms in this expression, which is the second step in the prescription, after we get the solutions for the Hamiltonian of equation (3).

In matrix form, we may write equation (3) as:

$$H_{rel} - E =$$

$$\begin{bmatrix} m_0c^2 - E - \frac{\lambda^2\hbar c}{m_0 c}\left(L_z + \frac{3}{2}\hbar\right) & 0 & p_z c - i\lambda^2(\hbar c)z & (p_x - ip_y)c + \lambda^2(\hbar c)(-ix - y) \\ 0 & m_0c^2 - E - \frac{\lambda^2(\hbar c)}{m_0 c}\left(L_z - \frac{3}{2}\hbar\right) & (p_x + ip_y)c + \lambda^2(\hbar c)(ix - y) & -p_z c - i\lambda^2 z \\ p_z c + i\lambda^2(\hbar c)z & (p_x - ip_y)c + \lambda^2(\hbar c)(-ix - y) & -m_0c^2 - E + \frac{\lambda^2(\hbar c)}{m_0 c}\left(L_z + \frac{3}{2}\hbar\right) & 0 \\ (p_x + ip_y)c + \lambda^2(\hbar c)(ix - y) & -p_z c + i\lambda^2(\hbar c)z & 0 & -m_0c^2 - E + \frac{\lambda^2(\hbar c)^2}{m_0 c}\left(L_z - \frac{3}{2}\hbar\right) \end{bmatrix}$$

Due to the nature of the term we add to the Hamiltonian of equation (1) to get equation (3), the form of the solutions of equation (3) can be deduced from those of equation (1):

$$(H_{rel} - E)\psi^{(+)} = (H_{rel} - E)\begin{bmatrix} a\,F_{pm}\phi_m\,u_{n_z} \\ b\,F_{p\,m+1}\phi_{m+1}\,u_{n_z+1} \\ c\,F_{pm}\phi_m\,u_{n_z+1} \\ d\,F_{p,m+1}\phi_{m+1}\,u_{n_z} \end{bmatrix} = 0 \qquad (7)$$

Combining equations (6) and (7), one gets equations to solve for a, b, c, d and a secular determinant of order 4 to solve for the energy eigenvalue E. These are

$$E = \pm\sqrt{m_0^2c^4 + 2\lambda^2(\hbar c)^2\left[2p + |m| + n_z + \frac{5}{2}\right] + \frac{\lambda^4(\hbar c)^4}{m_0^2c^4}\left(m^2 + m + \frac{5}{4}\right) \pm X} \qquad (8)$$

where $$X = 2\lambda^2(\hbar c)^2\sqrt{1 + \frac{2\lambda^2(\hbar c)^2}{m_0^2c^4}\left(2p + |m| + \frac{3}{2}\right) + \frac{\lambda^4(\hbar c)^4}{m_0^4c^8}\left(m^2 + m + \frac{1}{4}\right)} \qquad (9)$$

$$b = \frac{-4\sqrt{2}\,\frac{\lambda^4(\hbar c)^4}{m_0c^2}\sqrt{(p + m + 1)(n_z + 1)}}{DENOM}\,a \qquad (10)$$

$$c = \frac{-\sqrt{2}\, i\lambda (\hbar c)\sqrt{n_z+1}\; a}{\left\{-m_0c^2 - E + \frac{\lambda^2(\hbar c)^2}{m_0c^2}(m+\frac{3}{2})\right\}}\left[1 + \frac{8\lambda^4(\hbar c)^4}{m_0c^2}\frac{(p+m+1)}{DENOM}\right] \tag{11}$$

$$d = \frac{-2i\lambda(\hbar c)\sqrt{p+|m|+1}\; a}{\left\{-m_0c^2 - E + \frac{\lambda^2(\hbar c)^2}{m_0c^2}(m-\frac{1}{2})\right\}}\left[1 - \frac{4\frac{\lambda^4(\hbar c)^4}{m_0c^2}(n_z+1)}{DENOM}\right] \tag{12}$$

where

$$DENOM = \left[\left\{m_0c^2 - \frac{\lambda^2(\hbar c)^2}{m_0c^2}(m-\tfrac{1}{2})\right\}^2 + 4\lambda^2(\hbar c)^2\left(p+m+\frac{n_z}{2}+\frac{3}{2}\right) - E^2\right]\left\{-m_0^2 - E + \frac{\lambda^2(\hbar c)^2}{m_0c^2}(m+\tfrac{3}{2})\right\}$$

It is possible to check these solutions by another method, which is the diagonalization of the Hamiltonian of equation (3) in the basis of the solutions of equation (1). The same answers result.

One notices that, at first sight, there appears to be a zero point energy of $\frac{5}{2}\hbar\omega$ in equation (8). However, when one considers the nonrelativistic limits of the expressions (8) through (13), one finds that the actual zero point energy is $\frac{3}{2}\hbar\omega$. Part of this comes from the x in equation (8). For the upper sign in front of x, we get $\frac{7}{2}\hbar\omega$, and we find that b is much larger than a, c, or d. Hence, in the non-relativistic limit, the upper sign corresponds to a spin down solution. Since $m + 1$ and $n_z + 1$ occur in the second component of the solutions, the $\frac{7}{2}\hbar\omega$ really corresponds to $\frac{3}{2}\hbar\omega$. For the lower sign we get spin up solutions with the correct zero point energy.

We return now to the removal of the terms which violate spherical symmetry. If one expands equation (8) in a Taylor series, one gets

$$E_+ \cong m_0c^2 + \frac{\lambda^2(\hbar c)^2}{m_0c^2}\left[2p+|m|+n_z+\frac{5}{2}\right] \pm \frac{\lambda^2(\hbar c)^2}{m_0c^2} + \frac{\lambda^4(\hbar c)^4}{2m_0^3c^6}\left[(m^2+m+\frac{5}{4}) \pm 2\left(2p+|m|+\frac{3}{2}\right) \mp 2\left(2p+|m|+n_z+\frac{5}{2}\right) - \left(2p+|m|+n_z+\frac{5}{2}\right)^2 - 1\right] + O\left(\frac{\lambda^6(\hbar c)^6}{2m_0^5c^{10}}\right) \tag{14}$$

Comparing this equation with the Foldy-Wouthuysen transformation of equation (5), we find that the spherically symmetric Hamiltonian to this order is given by

$$H' = H - \frac{\lambda^4(\hbar c)^4}{2m_0^3c^6}\left(L_z \pm \tfrac{1}{2}\sigma_z\right)^2 + S_\pm \frac{\lambda^2(\hbar c)^2}{2m_0^3c^6}\left[p_z^2c^2 + \lambda^4(\hbar c)^2 z^2 + \lambda^2(\hbar c)^2 \beta_3 \sigma_z\right]$$
$$- S_\pm \frac{\lambda^2(\hbar c)^2}{2m_0^3c^6}\left[p^2c^2 + \lambda^4(\hbar c)^2 r^2 + \lambda^2(\hbar c)^2(1+\beta_3)\sigma_z\right] \qquad (15)$$

with eigenvalue

$$E' = E - \frac{\lambda^4(\hbar c)^4}{2m_0^3c^6}\left[m^2 + m + \tfrac{1}{4}\right] \pm \frac{\lambda^4(\hbar c)^4}{m_0^3c^6}(n_z+1) \mp \frac{\lambda^4(\hbar c)^4}{m_0^3c^6}\left[2p + |m| + n_z + \tfrac{5}{2}\right] \qquad (16)$$

where E is as in equation (8).

Having found a spherically symmetric Hamiltonian to this order, the next step is to consider $z_0 \neq 0$. One finds that the same procedure as above may be followed. To get a level ordering scheme that gives the correct spins and parities of nuclei for $z_0 = 0$, one adds the terms

$$H_{sp} = K(\hbar\omega)\left(2\vec{l}\cdot\vec{s} + \mu\left(\vec{l}^2 - \langle\vec{l}^2\rangle_{shell}\right)\right) \qquad (17)$$

to the above Hamiltonian, and uses numerical diagonalization of large matrices to obtain the new eigenvalues.

The relativistic problem differs from the non-relativistic one solved by Greiner, Scharnweber, Mosel (1) in that it is necessary to include the negative energy solutions in the basis of the matrix elements. There are non-vanishing matrix elements of $\vec{l}\cdot\vec{s}$ and $\vec{l}^2$ between positive and negative energy states.

The matrix elements of $\vec{\ell}\cdot\vec{s}$ and $\vec{\ell}^{\,2}$ can be calculated easily using the ladder relations given in Chapter III. For positive energy solutions, with odd functions of z in the top component, one finds:

$$
\begin{aligned}
(\psi_{p'm'n_z'}\,,\vec{\ell}\cdot\vec{s}\,\psi_{pmn_z}) &= a^*_{p'm'n_z'}a_{pmn_z}\left(\tfrac{1}{2}m\right)\delta_{p'p}\delta_{m'm}\delta_{n_z'n_z} \\
&+ b^*_{p'm'n_z'}a_{pmn_z}\left(-s_m\sqrt{2n_z\left(p+\tfrac{m+|m|}{2}+1\right)}\right)\delta_{p'p}\delta_{m'm}\frac{N^{n_z'+1}N^{n_z-1}\sqrt{2}\lambda z_0 D_{n_z'+1}D_{n_z-1}}{n_z'-n_z+2} \\
&+ \tfrac{1}{2}b^*_{p'm'n_z'}a_{pmn_z}\left(-s_m\sqrt{2(n_z+1)\left(p+\tfrac{|m|-m}{2}\right)}\right)\delta_{p'p-1}\delta_{m'm}\delta_{n_z'n_z} \\
&+ \tfrac{1}{2}a^*_{p'm'n_z'}b_{pmn_z}\left(-s_m\sqrt{2(n_z+1)\left(p+\tfrac{|m|-m}{2}+1\right)}\right)\delta_{p',p+1}\delta_{m'm}\delta_{n_z'n_z} \\
&+ a^*_{p'm'n_z'}b_{pmn_z}\left(-s_m\sqrt{p+\tfrac{m+|m|}{2}+1}\right)\delta_{p'p}\delta_{m'm}\frac{N^{n_z'}N^{n_z+1}}{\lambda(n_z'-n_z-2)}D'_{n_z'}(-\sqrt{2}\lambda z_0)D_{n_z+2}(-\sqrt{2}\lambda z_0) \\
&+ b^*_{p'm'n_z'}b_{pmn_z}\left(-\tfrac{1}{2}(m+1)\right)\delta_{p'p}\delta_{m'm}\delta_{n_z'n_z} \\
&+ c^*_{p'm'n_z'}c_{pmn_z}\left(\tfrac{1}{2}m\right)\delta_{p'p}\delta_{m'm}\delta_{n_z'n_z} \\
&+ c^*_{p'm'n_z'}d_{pmn_z}\left(-s_m\sqrt{2n_z\left(p+\tfrac{|m|-m}{2}+1\right)}\right)\delta_{p',p+1}\delta_{m'm}\frac{N^{n_z'+1}N^{n_z-1}\sqrt{2}\lambda z_0 D_{n_z'+1}D_{n_z-1}}{n_z'-n_z+2} \qquad (18) \\
&+ \tfrac{1}{2}c^*_{p'm'n_z'}d_{pmn_z}\left(-s_m\sqrt{2(n_z+1)\left(p+\tfrac{m+|m|}{2}+1\right)}\right)\delta_{p'p}\delta_{m'm}\delta_{n_z'n_z} \\
&+ \tfrac{1}{2}d^*_{p'm'n_z'}c_{pmn_z}\left(-s_m\sqrt{2(n_z+1)\left(p+\tfrac{m+|m|}{2}+1\right)}\right)\delta_{p'p}\delta_{m'm}\delta_{n_z'n_z} \\
&+ d^*_{p'm'n_z'}c_{pmn_z}\left(-s_m\sqrt{p+\tfrac{m-|m|}{2}}\right)\delta_{p',p-1}\delta_{m'm}\frac{N^{n_z'}N^{n_z+1}}{\lambda(n_z'-n_z+2)}D_{n_z'}D_{n_z+2}(-\sqrt{2}\lambda z_0) \\
&+ d^*_{p'm'n_z'}d_{pmn_z}\left(-\tfrac{1}{2}(m+1)\right)\delta_{p'p}\delta_{m'm}\delta_{n_z'n_z}
\end{aligned}
$$

$$
(\psi_{p'm'n_z'}\,,\vec{\ell}^{\,2}\,\psi_{pmn_z}) = a^*_{p'm'n_z'}a_{pmn_z}\left\{m^2+n_z(2p+|m|+2)+(n_z+1)(2p+|m|)\right\}\delta_{p'p}\,\delta_{n_z'n_z}\,\delta_{m'm} \qquad (19)
$$

$$+ b^{*}_{p'm'n_z'}\, b_{pmn_z}\Big\{(m+1)^2+(n_z+1)(2p+|m|+3)+(n_z+2)(2p+|m|+1)\Big\}\delta_{p'p}\,\delta_{m'm}\,\delta_{n_z'n_z}$$

$$+ c^{*}_{p'm'n_z'}\, c_{pmn_z}\Big\{m^2+(n_z+1)(2p+|m|+2)+(n_z+2)(2p+|m|)\Big\}\delta_{p'p}\delta_{m'm}\,\delta_{n_z'n_z}$$

$$+ d^{*}_{p'm'n_z'}\, d_{pmn_z}\Big\{(m+1)^2+n_z(2p+|m|+3)+(n_z+1)(2p+|m|+1)\Big\}\delta_{p'p}\delta_{m'm}\delta_{n_z'n_z}$$

$$+\delta_{p'p+1}\delta_{m'm}\Big[2\sqrt{2}\; a^{*}_{p'm'n_z'}\, a_{pmn_z}\, n_z(n_z-1)\sqrt{(p+1)(p+|m|+1)}\,\frac{N^{n_z'}N^{n_z}}{\lambda(n_z'-n_z+2)}\,D'_{n_z'}\,D_{n_z+2}$$

$$+4\sqrt{2}\,\lambda z_0\; b^{*}_{p'm'n_z'}\, b_{pmn_z}\sqrt{n_z(n_z+1)(p+1+\tfrac{1-5}{2})(p+|m|+1)}\,\frac{N^{n_z'+1}N^{n_z-1}}{n_z'-n_z+2}\,D_{n_z'+1}\,D_{n_z-1}$$

$$+4\sqrt{2}\,\lambda z_0\; c^{*}_{p'm'n_z'}\, c_{pmn_z}\sqrt{n_z(n_z+1)(p+1)(p+\tfrac{m+|m|}{2}+2)}\,\frac{N^{n_z'+1}N^{n_z-1}}{n_z'-n_z+2}\,D_{n_z'+1}\,D_{n_z-1}$$

$$+2\sqrt{2}\; d^{*}_{p'm'n_z'}\, d_{pmn_z}\, n_z(n_z-1)\sqrt{(p+1+\tfrac{1-5}{2})(p+|m|+1)}\,\frac{N^{n_z'}N^{n_z}}{\lambda(n_z'-n_z+2)}\,D'_{n_z'}\,D_{n_z+2}\Big]$$

$$+\delta_{p'p-1}\delta_{m'm}\Big[2\sqrt{2}\; a^{*}_{p'm'n_z'}\, a_{pmn_z}\sqrt{p(p+|m|)}\,\frac{N^{n_z'}N^{n_z}}{\lambda(n_z'-n_z-2)}\,D'_{n_z'}\,D_{n_z+2}$$

$$+2\sqrt{2}\; b^{*}_{p'm'n_z'}\, b_{pmn_z}\sqrt{(p+\tfrac{1-5}{2})(p+|m|+\tfrac{1-5}{2})}\,\frac{N^{n_z'+1}N^{n_z+1}}{\lambda(n_z'-n_z-2)}\Big[D'_{n_z'+1}\,D_{n_z+3}-D'_{n_z+3}\,D_{n_z'+1}\Big]$$

$$+2\sqrt{2}\; c^{*}_{p'm'n_z'}\, c_{pmn_z}\sqrt{p(p+|m|)}\,\frac{N^{n_z'+1}N^{n_z+1}}{\lambda(n_z'-n_z-2)}\Big[D'_{n_z'+1}\,D_{n_z+3}-D'_{n_z+3}\,D_{n_z'+1}\Big]$$

$$+2\sqrt{2}\; d^{*}_{p'm'n_z'}\, d_{pmn_z}\sqrt{(p+|m|)(p+\tfrac{1-5}{2})}\,\frac{N^{n_z'}N^{n_z}}{\lambda(n_z'-n_z-2)}\,D'_{n_z'}\,D_{n_z+2}\Big]$$

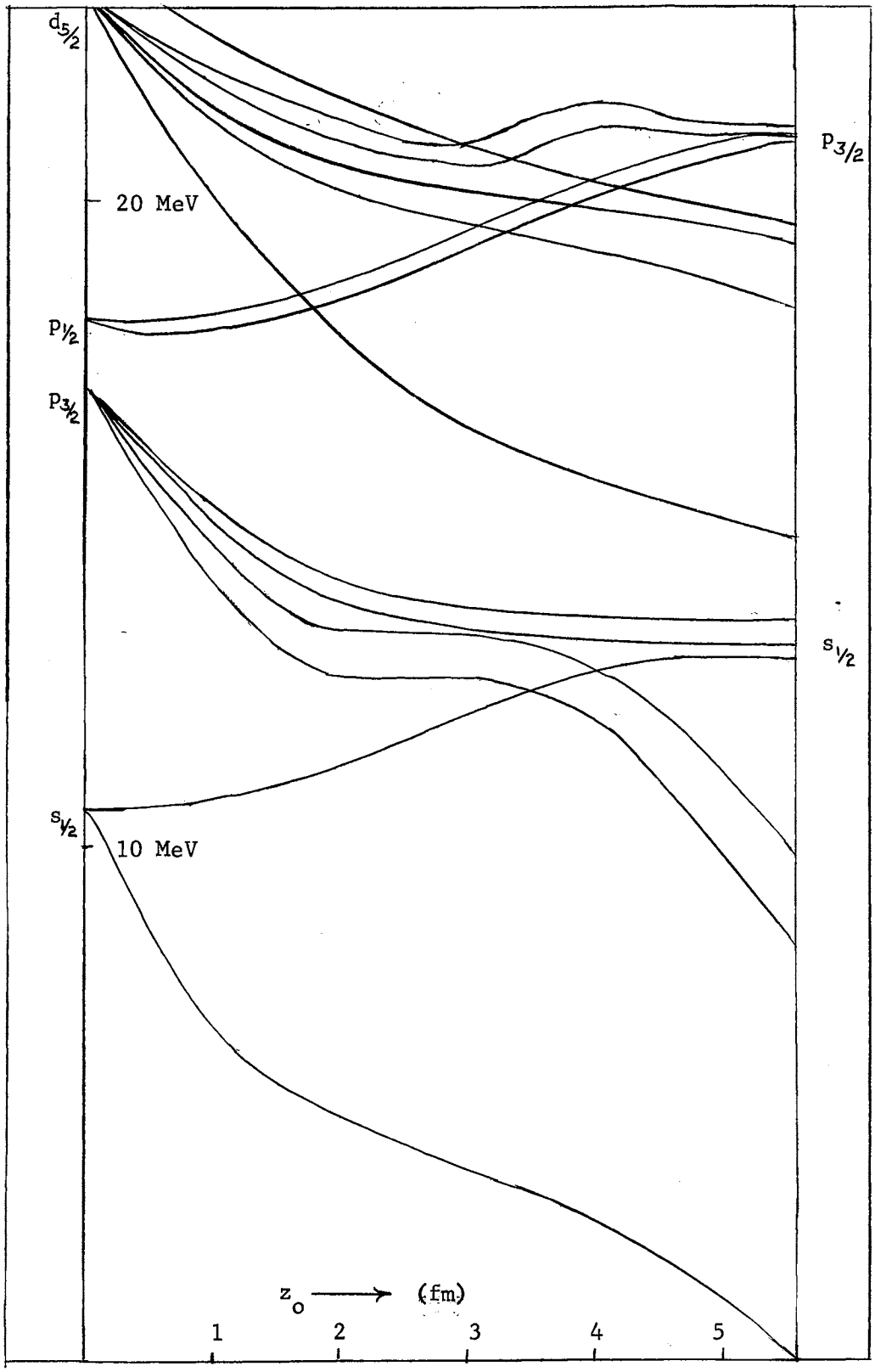

Figure 5. Energy Levels Calculated via the Present Model

To apply the above results to the calculation of the shell correction, one needs to put the volume conservation conditions to determine the oscillator constant, and use the linear relations discussed in Chapters IV and III to get mu and kappa. The energy levels which result for a nucleus in the lead region, calculated by diagonalization of a 224 by 224 matrix, are shown in Figure 5. The subroutine used to diagonalize this matrix was the SYMQR routine of Stewart (2).

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CHAPTER VI

SUMMARY

In the first part of this work, we discussed the relativistic covariance properties of the Dirac equation, and found that the relativistic equivalent oscillator in spherical coordinates corresponded to a Hermitian operator, which was introduced as a four-vector in the Dirac equation. We discussed the group theory of the equivalent oscillator, following the work of Chaffin (1). We then gave an enlargement of the non-invariance group to $SU(2,2) \times SU(2)$. A representation in the E^- series of Yao (2) was found to be applicable to the problem.

When we discussed the equivalent oscillator in cylindrical coordinates, it was found that certain modifications were necessary to satisfy the relativistic covariance requirements. We first performed a Foldy-Wouthuysen transformation of the Hamiltonian, and identified the terms which violated spherical symmetry when $z_0 = 0$. We then subtracted these terms from the Dirac Hamiltonian to obtain the new model. In the actual calculations, we did these subtractions through third order in $1/m_0$. They could, in principle, be carried out to higher order, although the extreme relativistic limit ($v = c$) could not be treated by this expansion method.

In Chapters III and IV we discussed the Strutinsky shell correction method (3). This method applies shell model energy levels to calculate

changes in the potential energy surface of a nucleus due to a high or low density of levels near the Fermi level, and provides a necessary clue to the interpretation of many recent experimental results. One version of calculation relies on the two center model of Greiner, Mosel, and Holzer (4).

This method uses a zero-order two center oscillator Hamiltonian which possesses exact solutions for all values of the separation of the two centers. The zero order Hamiltonian must be modified to give a level ordering for $z_0 = 0$ which matches the spins and parities of known nuclei, according to the shell model. This is done by adding spin orbit and orbital angular momentum squared type terms to the zero order Hamiltonian, in accordance with the method of Nilsson (5).

When we developed the two center Dirac equation, which had exact solutions for all values of the separations of the two centers, it was found that the potential became discontinuous at $z = 0$ for non-zero separations of the two centers of attraction. This led to different n_z quantum numbers from the non-relativistic case. For odd functions of z, the condition for determining n_z was found to be the same in the relativistic case as in the non-relativistic case, this condition being

$$D_{n_z}(-\sqrt{2}\lambda z_0) = 0.$$

For even functions of z, it was found that while the non-relativistic condition was

$$D'_{n_z}(-\sqrt{2}\lambda z_0) = 0,$$

the relativistic condition was that n_z should be an odd parity n_z value minus one. This led to a different behaviour of the equivalent oscillator solutions from the non-relativistic oscillator solutions for z_0 greater than zero.

Since a deformed nucleus has different properties from a spherical nucleus, one might expect the contributions of relativistic corrections to be larger. In recent years the theory of nuclear matter has been developed, and has shown that the mean free path of nucleons in nuclear matter is long compared to the size of real nuclei. This is one reason for the failure of the liquid drop model, since molecules in a liquid have a short mean free path. If one considers the constriction of the neck which occurs in nuclear fission, and the resulting constriction of the equipotentials, one might expect this constriction to "push" nucleons along, and lead in some fashion to larger relativistic corrections than those occuring in spherical nuclei. It is tempting to identify the effects of our discontinuous potential at $z = 0$ with these constriction of the neck type effects.

However, as z_0 approached infinity, it is found that the 1s level with an even function in the upper component approached $\frac{1}{2}\hbar\omega$ in energy. To get a proper asymptotic value of $\frac{3}{2}\hbar\omega$, we apparently need a new zero order Hamiltonian.

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APPENDIX A

PROGRAM FOR CALCULATION OF ENERGY LEVELS

This program, written in the FORTRAN language, calculates the energy levels of nucleons according to the model Hamiltonian. In the basis given by the solutions of the zero order Dirac Hamiltonian, the matrix elements of the additional spin-orbit, angular momentum squared, etc. terms are calculated. The number of states included in the matrix must be the same as the number of states which are included in the closed shells of the isotropic harmonic oscillator. The numbers NSHEL and N are thus related. For NSHEL = 5, N must be 224. The oscillator spacing, the number z_o, the constants mu and kappa, as well as the mass of the nucleons (protons or neutrons) must be supplied for each run. On the IBM 360/65 at Oklahoma State University, it was found that it takes 7 minutes 40 seconds to run the program. This program is for $z_0 \neq 0$.

```
C      PROGRAM FOR CALCULATING THE MATRIX ELEMENTS AND DIAGONALIZING
C      THE MATRIX.  THIS PROGRAM IS FOR ZO NOT EQUAL TO ZERO.
C      THE MAIN PART OF THE PROGRAM WAS WRITTEN BY EUGENE CHAFFIN.
C      THE SUBROUTINE SYMQR WAS BORROWED FROM PUBLISHED WORK OF G.W.
C      STEWART IN CACM.  THE PROGRAM WAS USED ON THE 360/65 AT OSU AND
C      USES DOUBLE PRECISION (REAL*8) VALUES FOR THE MATRIX ELEMENTS.
       REAL*8 ZO,XLAM,X
       REAL*8 D(224),EL(224),KO,EPS,AM(224,224)
       REAL*8 NZM1,NZP1,NZP2,NZP3,NZPP1,NZPM1,NZM2
       REAL*8 NZM3,NZPP2,NZPP3,NZPM2
       REAL*8 DD,DP,DERPN,DPN,ZNORM,F11,DGAM,DA
       REAL*8 NZTE,NZPTE
       INTEGER FAIL
       REAL*8 NZZ(7),NT,TEST
       REAL*8 A(4,3,11,6),B(4,3,11,6),C(4,3,11,6),D(4,3,11,6)
       REAL*8 MC2,E,F,G,H,DSQRT,DABS,DUM,DENOM,DEM
       REAL*8 EN,FN,P,M,NZ
       REAL*8 KAPPA,MJ,NTP,PP,MP,NZP,MAXP,DUM2,DUM3,DUM4,DUM5,DUM6,DUM7,
      1DUM8,DUM9
       REAL*8 YJ,DDD(3,7),ZNORR(8,7),DDP(8,7)
       LOGICAL ABSCNV,VEC,TRD
C      VEC HAS THE VALUE .FALSE. IF WE DO NOT WISH THE SUBROUTINE
C      SYMQR TO COMPUTE THE EIGENVECTORS.
       VEC=.FALSE.
C      ONE CHANGES THE SIZE OF THE MATRIX TO INCLUDE MORE SHELLS BY
C      DEFINING VALUES FOR N AND NSHEL.
       NSHEL=5
       N=224
       NA=N
       LLL=N
       MC2= 938.256D0
C      H  IS THE OSCILLATOR SPACING
       H= 7.75D0
       MJ= 0.6086D0
       KAPPA=0.36271D0
       ZO=2.45D0
C      X IS THE ARGUMENT OF THE Z DEPENDENT PART OF THE WAVE FUNCTION
C      FOR THE CASE Z=0.
       X=-1.5D0
C      XLAM IS THE OSCILLATOR CONSTANT LAMBDA
       XLAM=-X/(DSQRT(2.D0)*ZO)
       NZZ(1)=-0.79132669024832730
       NZZ(2)= 0.20867330975167300
       NZZ(3)= 0.64266582825960D0
       NZZ(4)= 1.64266582825960D0
       NZZ(5)= 2.20080282721751D0
       NZZ(6)= 3.20080282721751D0
       NZZ(7)=3.82943382751508D0
       DO 902 NI=1,8
       DO 902 NJ=1,7
       NIM1=NI-1
       IF(NIM1.EQ.0)NZ=-1.D0
       IF(NIM1.EQ.0)GO TO 901
       NZ=NZZ(NIM1)
  901  CONTINUE
       YJ=NJ
       IF(NJ.LE.4)NZ=NZ+YJ-1.D0
       IF(NJ.GT.4)NZ=NZ-YJ+4.D0
       DDD(NI,NJ)=DD(NZ,X)
```

```
      ZNORR(NI,NJ)=ZNORM(NZ,X,ZO)
      DDP(NI,NJ)=DP(NZ,X)
  902 CONTINUE
      L=0
C     THE MATRIX ELEMENTS ARE STORED IN AM(N,N)
C     INITIALIZE THE MATRIX ELEMENTS TO ZERO
      DO 500 LL=1,LLL
      DO 500 LP=1,LLL
      AM(LL,LP)= 0.D0
  500 CONTINUE
C     SET UP A LOOP WHICH GETS THE QUANTUM NUMBERS OF THE SOLUTIONS
C     PROCEEDING SHELL BY SHELL AND DEFINING THE LARGEST NEGATIVE M VALUE
C     WITHIN A SHELL FIRST.
C     IN THIS LOOP WE DEFINE PART OF THE DIAGONAL ELEMANTS OF THE MATRIX
C     AND FIND THE CONSTANTS A,B,C,D WHICH OCCUR IN THE DIFFERENT
C     COMPONENTS OF THE WAVEFUNCTION.
      IN=0
      NT= 0.D0
   10 M=-NT
      IM=-IN
   20 MAX=NT-DABS(M)
      IEVEN=IN-IABS(IM)
      IF(IEVEN.EQ.0)INZ=0
      IF(IEVEN.EQ.0)GO TO 29
      IEVEN=(-1)**IEVEN
      IF(IEVEN.LT.0)INZ=1
      IF(IEVEN.GT.0)INZ=0
   29 CONTINUE
      INZP1=INZ+1
      NZ=NZZ(INZP1)
   30 CONTINUE
      IP=(IN-INZ-IABS(IM))/2
      P=IP
      IF(M.LT.-0.1D0)J=IABS(IM)+6
      IF(M.GT.-0.1D0)J=IM+1
      I=IP+1
      K=INZ+1
    1 E= 1.D0+2.D0*(H/MC2)*( 2.DO*P+DABS(M)+NZ+2.5D0)+H*H*(M*M+M+1.25DO
     1)/(MC2*MC2)
      G= 1.D0+2.D0*(H/MC2)*( 2.DO*P+DABS(M)+1.5D0)+H*H*(M*M+M+0.25D0)/
     1(MC2*MC2)
      G=DSQRT(G)
      E= E-2.DO*(H/MC2)*G
      E= MC2*DSQRT(E)
      L=L+1
      AM(L,L)=E-H*H*(M*M+M+0.25DO)/( 2.DO*MC2)
      AM(L,L)=AM(L,L)+H*H*(2.D0*P+DABS(M)+1.5D0)/MC2
      AM(L,L)=AM(L,L)+KAPPA*H*MU* 0.5DO*NT*(NT+3.DO)
    3 A(1,I,J,K)= 1.D0
      DUM= 2.DO*(P+(M+DABS(M))/2.DO+1.DO)*(NZ+1.D0)
      DJM=-4.DO*H*H*MC2*DSQRT(DJM)
      DENOM=(((MC2-H*(M-0.5D0))**2+4.D0*H*MC2*(P+(M+DABS(M))/2.DO
     1+NZ/2.D0+1.5D0)-E*E)*(-MC2-E+H*(M+1.5D0))-8.D0*MC2*H*H*(P+(
     2M+DABS(M))/2.DO+1.DO))
      B(1,I,J,K)= DUM/DENOM
      IF(M.LT.-0.1DO)B(1,I,J,K)=-B(1,I,J,K)
      DUM= 2.DO*(NZ+1.DO)*MC2*H
      DUM=DSQRT(DUM)/(-MC2-E+H*(M+1.5D0))
      C(1,I,J,K)=-DUM*(1.D0+8.D0*MC2*H*H*(P+(M+DABS(M))/2.DO+1.DO)/
```

```
     1DENOM)
      DUM=(P+(M+DABS(M))/2.D0+1.D0)*MC2*H
      DJM= -2.D0*DSQRT(DUM)/(-MC2-E+H*(M-0.5D0))
      IF(M.LT. -0.1D0)DJM=-DJM
      D(1,I,J,K)= DUM*(1.D0-4.D0*MC2*H*H*(NZ+1.D0)/DENOM)
      DJM= 1.D0+B(1,I,J,K)**2+C(1,I,J,K)**2+D(1,I,J,K)**2
      DUM=DSQRT(DUM)
      A(1,I,J,K)= 1.D0/DUM
      B(1,I,J,K)= B(1,I,J,K)/DJM
      C(1,I,J,K)=C(1,I,J,K)/DUM


      D(1,I,J,K)=D(1,I,J,K)/DUM
      IF(IM.LE.0)P=P-1.D0
      M=M-1.D0
      IF(INZ.EQ.0)NZ=-1.D0
      IF(INZ.GT.0)NZ=NZZ(INZ)
      E= 1.D0+2.D0*(H/MC2)*( 2.D0*P+DABS(M)+NZ+2.5D0)+H*H*(M*M+M+1.25D0
     1)/(MC2*MC2)
      G= 1.D0+2.D0*(H/MC2)*( 2.D0*P+DABS(M)+1.5D0)+H*H*(M*M+M+0.25D0)/
     1(MC2*MC2)
      G=DSQRT(G)
      F= E+2.D0*(H/MC2)*G
      F=MC2*DSQRT(F)
    4 B(2,I,J,K)=-1.D0
      IF(M.LT.-0.1D0)B(2,I,J,K)=-B(2,I,J,K)
      DUM= 2.D0*(P+(M+DABS(M))/2.D0+1.D0)*(NZ+1.D0)
      DUM=-4.D0*H*H*MC2*DSQRT(DUM)
      DEM=(((MC2-H*(M+1.5D0))**2+4.D0*H*MC2*(P+(M+DABS(M))/2.D0+NZ/2.D0
     1+1.5D0)-F*F)*(-MC2-F+H*(M-0.5D0))+8.D0*MC2*H*H*(P+(M+DABS(M))/2.D0
     2+1.D0))
      A(2,I,J,K)=-DUM/DEM
      DUM= (P+(M+DABS(M))/2.D0+1.D0)*MC2*H
      DUM= -2.D0*DSQRT(DUM)/(-MC2-F+H*(M+1.5D0))
      C(2,I,J,K)= DJM*(1.D0+4.D0*MC2*H*H*(NZ+1.D0)/DEM)
      DUM= 2.D0*(NZ+1.D0)*MC2*H
      DUM=  DSQRT(DUM)/(-MC2-F+H*(M-0.5D0))
      IF(M.LT. -0.1D0)DUM=-DJM
      D(2,I,J,K)= DUM*(1.D0-8.D0*MC2*H*H*(P+(M+DABS(M))/2.D0+1.D0)/DEM)
      DJM= A(2,I,J,K)**2+1.D0+C(2,I,J,K)**2+D(2,I,J,K)**2
      DUM=DSQRT(DUM)
      A(2,I,J,K)=A(2,I,J,K)/DUM
      B(2,I,J,K)=B(2,I,J,K)/DUM
      C(2,I,J,K)=C(2,I,J,K)/DUM
      D(2,I,J,K)=D(2,I,J,K)/DUM
      L=L+1
      AM(L,L)=F-H*H*(M*M+M+0.25D0)/( 2.D0*MC2)
      AM(L,L)=AM(L,L)-H*H*(2.D0*P+DABS(M)+1.5D0)/MC2
      AM(L,L)=AM(L,L)+KAPPA*H*MJ* 0.5D0*NT*(NT+3.D0)
      M=M+1.D0
      IF(IM.LE.0)P=P+1.D0
      E= 1.D0+2.D0*(H/MC2)*( 2.D0*P+DABS(M)+NZ+2.5D0)+H*H*(M*M+M+1.25D0
     1)/(MC2*MC2)
      G= 1.D0+2.D0*(H/MC2)*( 2.D0*P+DABS(M)+1.5D0)+H*H*(M*M+M+0.25D0)/
     1(MC2*MC2)
      G=DSQRT(G)
      E=E-2.D0*(H/MC2)*G
      E= MC2*DSQRT(E)
      EN=-E
```

```
      L=L+1
      AM(L,L)=EN+H*H*(M*M+M+0.25D0)/( 2.D0*MC2)
      AM(L,L)=AM(L,L)-H*H*(2.D0*P+DABS(M)+1.5D0)/MC2
      AM(L,L)=AM(L,L)+KAPPA*H*MU* 0.5D0*NT*(NT+3.D0)
    5 C(3,I,J,K)=-1.D0
      DUM= 2.D0*(P+(M+DABS(M))/2.D0+1.D0)*(NZ+1.D0)
       DUM= 4.D0*H*H*MC2*DSQRT(DUM)
      DENOM=(((MC2-H*(M-0.5D0))**2+4.D0*H*MC2*(P+(M+DABS(M))/2.D0
     1+NZ/2.D0+1.5D0)-EN*EN)*( MC2-EN-H*(M+1.5D0))+8.D0*MC2*H*H*(P+(
     2M+DABS(M))/2.D0+1.D0))
      D(3,I,J,K)= DUM/DENOM
      IF(M.LT.-0.1D0)D(3,I,J,K)=-D(3,I,J,K)
      DUM= 2.D0*(NZ+1.D0)*MC2*H
      DUM= DSQRT(DUM)/( MC2-EN-H*(M+1.5D0))
      A(3,I,J,K)= DUM*( 1.D0-8.D0*MC2*H*H*(P+(M+DABS(M))/2.D0+1.D0)
     1/DENOM)
      DUM= (P+(M+DABS(M))/2.D0+1.D0)*MC2*H
      DUM=  2.D0*DSQRT(DUM)/( MC2-EN-H*(M-0.5D0))
      IF(M.GT.-0.1D0)DUM=-DUM
      B(3,I,J,K)= DUM*( 1.D0+4.D0*MC2*H*H*(NZ+1.D0)/DENOM)
      DUM= A(3,I,J,K)**2+B(3,I,J,K)**2+1.D0+D(3,I,J,K)**2
      DUM=DSQRT(DUM)
      A(3,I,J,K)=A(3,I,J,K)/DUM
      B(3,I,J,K)=B(3,I,J,K)/DUM
      C(3,I,J,K)=C(3,I,J,K)/DUM
      D(3,I,J,K)=D(3,I,J,K)/DUM
      IF( IM.LE.0)P=P-1.D0
      M=M-1.D0
      NZ=NZZ(INZP1)
      E= 1.D0+2.D0*(H/MC2)*( 2.D0*P+DABS(M)+NZ+2.5D0)+H*H*(M*M+M+1.25D0
     1)/(MC2*MC2)
      G= 1.D0+2.D0*(H/MC2)*( 2.D0*P+DABS(M)+1.5D0)+H*H*(M*M+M+0.25D0)/
     1(MC2*MC2)
      G=DSQRT(G)
      F=E+2.D0*(H/MC2)*G
      F=MC2*DSQRT(F)
      FN=-F
      L=L+1
      AM(L,L)=FN+H*H*(M*M+M+0.25D0)/( 2.D0*MC2)
      AM(L,L)=AM(L,L)+H*H*(2.D0*P+DABS(M)+1.5D0)/MC2
      AM(L,L)=AM(L,L)+KAPPA*H*MU* 0.5D0*NT*(NT+3.D0)
    6 D(4,I,J,K)=-1.D0
      IF(M.LT.-0.1D0)D(4,I,J,K)=-D(4,I,J,K)
      DUM= 2.D0*(P+(M+DABS(M))/2.D0+1.D0)*(NZ+1.D0)
       DUM= 4.D0*H*H*MC2*DSQRT(DUM)
      DEM  =(((MC2-H*(M+1.5D0))**2+4.D0*H*MC2*(P+(M+DABS(M))/2.D0
     1+NZ/2.D0+1.5D0)-FN*FN)*( MC2-FN-H*(M-0.5D0))-8.D0*MC2*H*H*(P+(
     2M+DABS(M))/2.D0+1.D0))
      C(4,I,J,K)= DUM/DEM
      DUM= 2.D0*(NZ+1.D0)*MC2*H
      DUM=DSQRT(DUM)/( MC2-FN-H*(M-0.5D0))
      DUM=-DUM
      IF(M.GT.-0.1D0)DUM=-DUM
      B(4,I,J,K)= DUM*( 1.D0+8.D0*MC2*H*H*(P+(M+DABS(M))/2.D0+1.D0)/DEM)
      DUM= (P+(M+DABS(M))/2.D0+1.D0)*MC2*H
      DUM=-2.D0*DSQRT(DUM)/( MC2-FN-H*(M+1.5D0))
      DUM=-DUM
      A(4,I,J,K)=DJM*(1.D0-4.D0*MC2*H*H*(NZ+1.D0)/DEM)
      DUM= A(4,I,J,K)**2+B(4,I,J,K)**2+C(4,I,J,K)**2+1.D0
```

```
      DUM=DSQRT(DUM)
      A(4,I,J,K)=A(4,I,J,K)/DUM
      B(4,I,J,K)= B(4,I,J,K)/DUM
      C(4,I,J,K)=C(4,I,J,K)/DUM
      D(4,I,J,K)=D(4,I,J,K)/DUM
    7 CONTINUE
      M=M+1.D0
      IF(IM.LE.0)P=P+1.D0
      NZTE=INZ
      TEST=MAX-NZTE
      TEST=DABS(TEST)
      IF(TEST.LT. 1.D-03)GO TO 40
      INZ=INZ+2
      INZP1=INZ+1
      NZ=NZZ(INZP1)
      GO TO 30
   40 TEST=NT-M
      TEST=DABS(TEST)
      IF(TEST.LT. 1.D-03)GO TO 50
      M=M+1.D0
      IM=IM+1
      GO TO 20
   50 NT=NT+1.D0
      IN=IN+1
      IF(IN.LE.NSHEL)GO TO 10
C     WE NOW SET UP TWO NESTED LOOPS INSIDE WHICH PRIMED AND
C     UNPRIMED QUANTUM NUMBERS ARE DEFINED CORRESPONDING TO
C     THE TWO WAVEFUNCTIONS OF A GIVEN MATRIX ELEMENT
C     WHEN THESE QUANTUM NUMBERS ARE DEFINED, WE PROCEED TO GO THROUGH
C     AND CHECK TO SEE IF VARIOUS KRONECKER DELTAS ARE ZERO, AND
C     TO INCLUDE THE CONTRIBUTIONS OF THE VARIOUS TERMS IN THE MATRIX.
C      ONLY THE LOWER TRIANGLE OF THE MATRIX IS DEFINED, SINCE THIS ALL
C     THAT SYMOR REQUIRES FOR THIS SYMMETRIC MATRIX.
      IL=0
      JL=0
      IN=0
      NT= 0.D0
  110 M=-NT
      IM=-IN
  120 MAX=NT-DABS(M)
      IEVEN=IN-IABS(IM)
      IF(IEVEN.EQ.0)INZ=0
      IF(IEVEN.EQ.0)GO TO 129
      IEVEN=(-1)**IEVEN
      IF(IEVEN.LT.0)INZ=1
      IF(IEVEN.GT.0)INZ=0
  129 CONTINUE
      INZP1=INZ+1
      NZ=NZZ(INZP1)
  130 CONTINUE
      IP=(IN-INZ-IABS(IM))/2
      P=IP
      IF(M.LT.-0.1D0)J=IABS(IM)+6
      IF(M.GT.-0.1D0)J=IM+1
      I=IP+1
      K=INZ+1
      DO 139 IS=1,4
      JL=JL+1
      IL=JL
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```
      NTP=NT
      INP=IN
      PP=P
      MP=M
      NZP=NZ
      MAXP=MAX
      INZP=INZ
      IMP=IM
      IPP=IP
      ISP=IS
      IIP=I
      JP=J
      KP=K
      GO TO 235
  210 MP=-NTP
      IMP=-INP
  220 MAXP=NTP-DABS(MP)
      IEVENP=INP-IABS(IMP)
      IF(IEVENP.EQ.0)INZP=0
      IF(IEVENP.EQ.0)GO TO 229
      IEVENP=(-1)**IEVENP
      IF(IEVENP.LT.0)INZP=1
      IF(IEVENP.GT.0)INZP=0
  229 CONTINUE
      INZPP1=INZP+1
      NZP=NZZ(INZPP1)
  230 CONTINUE
      IPP=(INP-INZP-IABS(IMP))/2
      PP=IPP
      IF(MP.LT.-0.1D0)JP=IABS(IMP)+6
      IF(MP.GT.-0.1D0)JP=IMP+1
      IIP=IPP+1
      KP=INZP+1
      ISP= 1
  235 CONTINUE
      IF(IS.EQ.2.AND.IM.LE.0)P=P-1.D0
      IF(IS.EQ.4.AND.IM.LE.0)P=P-1.D0
      IF(IS.EQ.2.OR.IS.EQ.4)M=M-1.D0
      IF(IS.EQ.2.AND.INZ.EQ.0)NZ=-1.D0
      IF(IS.EQ.3.AND.INZ.EQ.0)NZ=-1.D0
      IF(IS.EQ.2.AND.INZ.GT.0)NZ=NZZ(INZ)
      IF(IS.EQ.3.AND.INZ.GT.0)NZ=NZZ(INZ)
      IF(ISP.EQ.2.AND.IMP.LE.0)PP=PP-1.D0
      IF(ISP.EQ.4.AND.IMP.LE.0)PP=PP-1.D0
      IF(ISP.EQ.2.OR.ISP.EQ.4)MP=MP-1.D0
      IF(ISP.EQ.2.AND.INZP.EQ.0)NZP=-1.D0
      IF(ISP.EQ.2.AND.INZP.GT.0)NZP=NZZ(INZP)
      IF(ISP.EQ.3.AND.INZP.EQ.0)NZP=-1.D0
      IF(ISP.EQ.3.AND.INZP.GT.0)NZP=NZZ(INZP)
      IF(IS.EQ.2.AND.IM.LE.0)IP=IP-1
      IF(IS.EQ.4.AND.IM.LE.0)IP=IP-1
      IF(IS.EQ.2.OR.IS.EQ.4)IM=IM-1
      IF(IS.EQ.2.OR.IS.EQ.3)INZ=INZ-1
      IF(ISP.EQ.2.AND.IMP.LE.0)IPP=IPP-1
      IF(ISP.EQ.4.AND.IMP.LE.0)IPP=IPP-1
      IF(ISP.EQ.2.OR.ISP.EQ.4)IMP=IMP-1
      IF(ISP.EQ.2.OR.ISP.EQ.3)INZP=INZP-1
      NI=INZ+2
      IF(NZ.LT.-0.999999D0)NI=1
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```
      NJ=1
      NJP1=NJ+1
      NJP2=NJ+2
      NJP3=NJ+3
      NJM1=NJ+4
      NJM2=NJ+5
      NJM3=NJ+6
      NIP=INZP+2
      IF(NZP.LT.-0.999999D0)NIP=1
      NJP=1
      NJPP1=NJP+1
      NJPP2=NJP+2
       NJPP3=NJP+3
      NJPM1=NJP+4
      NJPM2=NJP+5
      NJPM3=NJP+6
      IF(INZ.EQ.0)IPAR=1
      IF(INZP.EQ.0)GO TO 799
      IPARP=(-1)**INZP
      IF(INZ.EQ.0)GO TO 800
  799 IF(INZP.EQ.0)IPARP=1
      IF(INZ.EQ.0)GO TO 800
      IPAR=(-1)**INZ
  800 CONTINUE
      IF(NZ.LT.-0.999D0)IPAR=-1
      IF(NZP.LT.-0.999D0)IPARP=-1
      IF(IPAR.NE.IPARP)GO TO 316
      IF(IM.NE.IMP)GO TO 316
      NZP1=NZ+1.D0
      NZP2=NZ+2.D0
      NZP3=NZ+3.D0
      NZM1=NZ-1.D0
      NZPP1=NZP+1.D0
       NZPM1=NZP-1.D0
      DUM=2.D0*(NZ+1.D0)*(P+(M+DABS(M))/2.D0+1.D0)
      DUM=DSQRT(DUM)
      IF(M.GT.-0.1D0)DUM=-DUM
      IF(INZ.NE.INZP.OR.IP.NE.IPP.OR.IM.NE.IMP)GO TO 400
C     DIAGONAL AND (SPIN DOWN,SPIN UP), ETC. TYPE ELEMENTS OF L.S
      DEM=A(ISP,IIP,JP,KP)*A(IS,I,J,K)*M-B(ISP,IIP,JP,KP)*B(IS,I,J,K)*(
     1M+1.D0)+C(ISP,IIP,JP,KP)*C(IS,I,J,K)*M-D(ISP,IIP,JP,KP)*
     2D(IS,I,J,K)*(M+1.D0)+C(ISP,IIP,JP,KP)*D(IS,I,J,K)*DUM+D(ISP,IIP,
     3JP,KP)*C(IS,I,J,K)*DJM
      DEM= 0.5*DEM
      DEM= KAPPA*H*2.D0*DEM
      AM(IL,JL)=AM(IL,JL)-DEM
C     DIAGONAL AND(SPIN DOWN,SPIN UP), ETC. TYPE ELEMENTS OF L.L
      DEM=A(ISP,IIP,JP,KP)*A(IS,I,J,K)*(M*M+NZ*(2.D0*P+DABS(M)+2.D0)
     1+(NZ+1.D0)*(2.D0*P+DABS(M)))+B(ISP,IIP,JP,KP)*B(IS,I,J,K)*((M+1.D0
     2)*(M+1.D0)+(NZ+1.D0)*(2.D0*P+DABS(M)+3.D0)+(NZ+2.D0)*(2.D0*P+
     3DABS(M)+1.D0)) +C(ISP,IIP,JP,KP)*C(IS,I,J,K)*(M*M+(NZ+1.D0)*(2.D0
     4*P+DABS(M)+2.D0)+(NZ+2.D0)*(2.D0*P+DABS(M)))+D(ISP,IIP,JP,KP)*
     5D(IS,I,J,K)*((M+1.D0)*(M+1.D0)+NZ*(2.D0*P+DABS(M)+3.D0)+(NZ+1.D0)
     6*(2.D0*P+DABS(M)+1.D0))
      DEM=KAPPA*MU*H*DEM
      AM(IL,JL)=AM(IL,JL)-DEM
  400 CONTINUE
      NZP1=NZ+1.D0
      NZP2= NZ+2.D0
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      NZM1=NZ-1.D0
      NZM2=NZ-2.D0
      NZPP1=NZP+1.D0
      IF(IP.NE.IPP.OR.IM.NE.IMP)GO TO 405
      IF(IPAR.GT.0)GO TO 888
      DEM=B(ISP,IIP,JP,KP)*B(IS,I,J,K)*2.D0*(2.D0*P+DABS(M)+1.D0)*
     1ZNORR(NIP,NJPP1)*ZNORR(NI,NJP1)*DDD(NIP,NJPP1)*DDD(NI,NJP2)
      DEM=DEM+C(ISP,IIP,JP,KP)*C(IS,I,J,K)*2.D0*(2.D0*P+DABS(M))*
     1ZNORR(NIP,NJPP1)*ZNORR(NI,NJP1)*DDD(NIP,NJPP1)*DDD(NI,NJP2)
      GO TO 401
  888 CONTINUE
      DEM=A(ISP,IIP,JP,KP)*A(IS,I,J,K)*(-2.D0)*NZ*(2.D0*P+DABS(M)+2.D0)
     1*ZNORR(NIP,NJP)*ZNORR(NI,NJ)*DDD(NIP,NJP)*DDD(NI,NJM1)
      DEM=DEM+D(ISP,IIP,JP,KP)*D(IS,I,J,K)*(-2.D0)*NZ*(2.D0*P+DABS(M)
     1+3.D0)*ZNORR(NIP,NJP)*ZNORR(NI,NJ)*DDD(NIP,NJP)*DDD(NI,NJM1)
  401 CONTINUE
C     PP,P  MP,M  MZP,NZ+2  TERM OF L.S
      DUM2=P+(M+DABS(M))/2.D0+1.D0
      IF(DUM2.LT.0.D0)DUM2= 0.D0
      DUM2=DSQRT(DUM2)
      IF(M.GT.-0.1D0)DUM2=-DUM2
      IF(IP.NE.IPP.OR.IM.NE.IMP)GO TO 405
      INZP2=INZ+2
      IF(IPAR.GT.0)GO TO 402
      AM(IL,JL)=AM(IL,JL)-2.D0*KAPPA*H*DUM2*ZNORR(NIP,NJP)*ZNORR(NI,
     1NJP1)*DDP(NIP,NJP)*DDD(NI,NJP2)*A(ISP,IIP,JP,KP)*B(IS,I,J,K)/(
     2XLAM*(NZP-NZ-2.D0))
      GO TO 403
  402 CONTINUE
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*DUM2*X*ZNORR(NIP,NJP)*ZNORR(NI,NJP1)*
     12.D0*(1.4142135624013700)*A(ISP,IIP,JP,KP)*B(IS,I,J,K)*DDD(NIP
     2,NJP)*DDD(NI,NJP2)/(NZP-NZ-2.D0)
  403 CONTINUE
C     PP,P MP,M MZP,NZ-2 TERM OF L.S
      DUM3= 2.D0*NZ*(P+(M+DABS(M))/2.D0+1.D0)
      IF(DUM3.LT.0.D0)DUM3= 0.D0
      DUM3=DSQRT(DUM3)
      IF(M.GT.-0.1D0)DUM3=-DUM3
      INZM2=INZ-2
      IF(IPAR.GT.0)GO TO 404
      AM(IL,JL)=AM(IL,JL)-(-2.D0)*KAPPA*H*DUM3*B(ISP,IIP,JP,KP)*
     1A(IS,I,J,K)*ZNORR(NI,NJM1)*ZNORR(NIP,NJPP1)*X*DDD(NIP,NJPP1)*
     2DDD(NI,NJM1)/(NZP-NZ+2.D0)
      GO TO 405
  404 CONTINUE
      DUM3= 2.D0*(P+(M+DABS(M))/2.D0+1.D0)
      IF(DUM3.LT. 0.D0)DUM3= 0.D0
      DUM3=NZ*DSQRT(DUM3)
      IF(M.GT.-0.1D0)DUM3=-DUM3
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*B(ISP,IIP,JP,KP)*A(IS,I,J,K)*DUM3*
     12.D0*ZNORR(NIP,NJPP1)*ZNORR(NI,NJ)*DDP(NIP,NJPP1)*DDD(NI,NJM1)/(
     2XLAM*(NZP-NZ+2.D0))
  405 CONTINUE
C     PP,P-1 MP,M MZP,NZ TERM OF L.S
      IPM1=IP-1
      IF(IPP.NE.IPM1.OR.IMP.NE.IM.OR.INZ.NE.INZP)GO TO 407
      DUM4= 2.D0*(NZ+1.D0)*(P+(DABS(M)-M)/2.D0)
      IF(DUM4.LT.0.D0)DUM4= 0.D0
      DUM4= DSQRT(DUM4)
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      IF(M.GT.-0.1D0)DUM4=-DJM4
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*B(ISP,IIP,JP,KP)*A(IS,I,J,K)*DUM4
  407 CONTINUE
C     PP,P+1 MP,M NZP,NZ TERM OF L .S
      IPP1=IP+1
      IF(IPP.NE.IPP1.OR.IMP.NE.IM.OR.INZ.NE.INZP)GO TO 409
      DUM5= 2.D0*(NZ+1.D0)*(P+(DABS(M)-M)/2.D0+1.D0)
      IF(DUM5.LT.0.D0)DUM5= 0.D0
      DUM5=DSQRT(DUM5)
      IF(M.GT.-0.1D0)DUM5=-DUM5
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*A(ISP,IIP,JP,KP)*B(IS,I,J,K)*DUM5
  409 CONTINUE
C     PP,P+1 MP,M NZP,NZ-2 TERM OF L.S
      IPP1=IP+1
      INZM2=INZ-2
      IF(IPP.NE.IPP1.OR.IMP.NE.IM)GO TO 412
      IF(IPAR.GT.0)GO TO 410
      DUM6= 2.D0*NZ*(P+(DABS(M)-M)/2.D0+1.D0)
      IF(DUM6.LT.0.D0)DUM6= 0.D0
      DUM6=DSQRT(DUM6)
      IF(M.GT.-0.1D0)DUM6=-DJM6
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*C(ISP,IIP,JP,KP)*D(IS,I,J,K)*DUM6*
     12.D0*ZNORR(NIP,NJPP1)*ZNORR(NI,NJM1)*(-X)*DDD(NIP,NJPP1)*
     2DDD(NI,NJM1)/(NZP-NZ+2.D0)
      GO TO 411
  410 CONTINUE
      DUM6= 2.D0*(P+(DABS(M)-M)/2.D0+1.D0)
      IF(DUM6.LT.0.D0)DUM6= 0.D0
      DUM6=DSQRT(DUM6)
      DUM6=NZ*DUM6
      IF(M.GT.-0.1D0)DJM6=-DJM6
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*C(ISP,IIP,JP,KP)*D(IS,I,J,K)*DUM6*
     12.D0*ZNORR(NIP,NJPP1)*ZNORR(NI,NJ)*DDP(NIP,NJPP1)*DDD(NI,NJM1)/(
     2XLAM*(NZP-NZ+2.D0))
  411 CONTINUE
C     PP,P+1 MP,M NZP,NZ-2  AND  PP,P+1 MP,M NZP+1,NZ-1 TERMS OF L.L
      IF(IPP.NE.IPP1.OR.IMP.NE.IM)GO TO 412
      IF(IPAR.GT.0)GO TO 889
      DUM7=(P+1.D0)*(P+DABS(M)+1.D0)
      IF(DUM7.LT.0.D0)DUM7= 0.D0
      DUM7= 2.D0*DSQRT(2.D0)*NZ*(NZ-1.D0)*DSQRT(DUM7)
      DEM=DJM7*A(ISP,IIP,JP,KP)*A(IS,I,J,K)*ZNORR(NIP,NJP)*ZNORR(NI,NJ)*
     1DDP(NIP,NJP)*DDD(NI,NJP2)/(XLAM*(NZP-NZ+2.D0))
      DUM7= P+2.D0
      IF(M.GT.-0.1D0)DUM7=DUM7-1.D0
      DUM7=DUM7*NZ*(NZ+1.D0)*(P+DABS(M)+1.D0)
      DUM7= 4.D0*(-X)*DSQRT(DUM7)
      DEM=DEM+DJM7*ZNORR(NIP,NJPP1)*ZNORR(NI,NJM1)*B(ISP,IIP,JP,KP)*
     1B(IS,I,J,K)*DDD(NIP,NJPP1)*DDD(NI,NJM1)/(NZP-NZ+2.D0)
      DJM7=NZ*NZP1*(P+1.D0)*(P+(M+DABS(M))/2.D0+2.D0)
      IF(DUM7.LT.0.D0)DUM7=0.D0
      DUM7= 4.D0*(-X)*DSQRT(DUM7)
      DEM=DEM+C(ISP,IIP,JP,KP)*C(IS,I,J,K)*DJM7*ZNORR(NIP,NJPP1)*
     1ZNORR(NI,NJM1)*DDD(NIP,NJPP1)*DDD(NI,NJM1)/(NZP-NZ+2.D0)
      DUM7=P+2.D0
      IF(M.GT.-0.1D0)DUM7=DUM7-1.D0
      DUM7=DUM7*(P+DABS(M)+1.D0)
      DJM7= 2.D0*DSQRT(2.D0)*NZ*(NZ-1.D0)*DSQRT(DUM7)
      DEM=DEM+D(ISP,IIP,JP,KP)*D(IS,I,J,K)*DUM7*ZNORR(NIP,NJP)*
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     1ZNORR(NI,NJ)*DDP(NIP,NJP)*DDD(NI,NJP2)/(XLAM*(NZP-NZ+2.D0))
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*MU*DEM
      GO TO 412
  889 CONTINUE
      DUM7=(P+1.D0)*(P+DABS(M)+1.D0)
      IF(DUM7.LT.0.D0)DUM7= 0.D0
      DUM7=DSQRT(DUM7)*NZ*(NZ-1.D0)*2.D0*DSQRT(2.D0)
      DEM=DUM7*A(ISP,IIP,JP,KP)*A(IS,I,J,K)*ZNORR(NIP,NJP)*ZNORR(NI,NJ)*
     1(DDP(NIP,NJP)*DDD(NI,NJM2)-DDP(NI,NJM2)*DDD(NIP,NJP))/(XLAM*
     2(NZP-NZ-2.D0))
      DUM7= P+2.D0
      IF(M.GT.-0.1D0)DUM7=DUM7-1.D0
      DUM7=DUM7*2.D0*(P+DABS(M)+1.D0)
      IF(DUM7.LT.0.D0)DUM7= 0.D0
      DUM7= NZ*NZP1*DSQRT(DUM7)*2.D0
      DEM=DEM+DUM7*B(ISP,IIP,JP,KP)*B(IS,I,J,K)*ZNORR(NIP,NJPP1)*
     1ZNORR(NI,NJP1)*DDP(NIP,NJPP1)*DDD(NI,NJM1)/(XLAM*(NZP-NZ-2.D0))
      DUM7= (P+1.D0)*(P+DABS(M)+1.D0)*2.D0
      IF(DUM7.LT.0.D0)DUM7= 0.D0
      DUM7= 2.D0*NZ*NZP1*DSQRT(DUM7)
      DEM=DEM+DUM7*C(ISP,IIP,JP,KP)*C(IS,I,J,K)*ZNORR(NIP,NJPP1)*
     1ZNORR(NIP,NJPP1)*DDP(NI,NJP1)*DDD(NI,NJM1)/(XLAM*(NZP-NZ-2.D0))
      DUM7= P+2.D0
      IF(M.GT.-0.1D0)DUM7=DUM7-1.D0
      DUM7=DUM7*(P+DABS(M)+1.D0)*2.D0
      IF(DUM7.LT.0.D0)DUM7= 0.D0
      DUM7=NZ*(NZ+1.D0)*DSQRT(DUM7)*2.D0
      DEM=DEM+DUM7*D(ISP,IIP,JP,KP)*D(IS,I,J,K)*ZNORR(NIP,NJP)*
     1ZNORR(NI,NJ)*(DDP(NIP,NJPP1)*DDD(NI,NJM2)-DDP(NI,NJM2)*
     2DDD(NIP,NJP))/(XLAM*(NZP-NZ-2.D0))
      DUM7= (P+1.D0)*(P+DABS(M)+1.D0)
      IF(DUM7.LT.0.D0)DUM7= 0.D0
      DUM7= 2.D0*NZ*DSQRT(DUM7)
      DUM7= P+ 2.D0
      IF(M.GT.-0.1D0)DUM7=DUM7-1.D0
      DUM7=DUM7*(P+DABS(M)+2.D0)
      IF(DUM7.LT.0.D0)DUM7= 0.D0
      DUM7= 2.D0*NZ*DSQRT(DUM7)
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*MU*DEM
  412 CONTINUE
C     PP,P-1 MP,M NZP,NZ+2  TERM OF L.S
      IPM1=IP-1
      INZP2=INZ+2
      IF(IPP.NE.IPM1.OR.IMP.NE.IM)GO TO 415
      IF(IPAR.GT.0)GO TO 414
      DUM8=P+(DABS(M)-M)/2.D0
      IF(DUM8.LT.0.D0)DUM8=0.D0
      DUM8=DSQRT(DUM8)
      IF(M.LT.-0.1D0)DUM8=-DUM8
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*D(ISP,IIP,JP,KP)*C(IS,I,J,K)*DUM8*
     12.D0*ZNORR(NIP,NJP)*ZNORR(NI,NJP1)*DDD(NIP,NJP)*DDD(NI,NJP2)/(
     2XLAM*(NZP-NZ-2.D0))
      GO TO 413
  414 CONTINUE
      DUM8= 2.D0*(NZ+2.D0)*(P+(DABS(M)-M)/2.D0)
      IF(DUM8.LT.0.D0)DUM8=0.D0
      DUM8=DSQRT(DUM8)*(-X)*2.D0
      IF(M.GT.-0.1D0)DUM8=-DUM8
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*D(ISP,IIP,JP,KP)*C(IS,I,J,K)*DJM8*
```

```
     1ZNORR(NIP,NJP)*ZNORR(NI,NJP2)*DDD(NIP,NJP)*DDD(NI,NJP2)/(NZP-NZ
     2-2.D0)
  413 CONTINUE
C      PP,P-1 MP,M NZP,NZ+2 AND PP,P-1 MP,M NZP+1,NZ+3 TERMS OF L.L
       IF(IPP.NE.IPM1.OR.IMP.NE.IM)GO TO 415
       IF(IPAR.GT.0)GO TO 887
       DUM9= P*(P+DABS(M))*2.D0
       IF(DUM9.LT.0.D0)DUM9= 0.D0
       DUM9=DSQRT(DUM9)*2.D0
       DEM=DUM9*A(ISP,IIP,JP,KP)*A(IS,I,J,K)*ZNORR(NIP,NJP)*ZNORR(NI,NJ)
     1*DDP(NIP,NJP)*DDD(NI,NJP2)/(XLAM*(NZP-NZ-2.D0))
       DUM9= P+1.D0
       IF(M.GT.-0.1D0)DUM9=DUM9-1.D0
       DUM9=DUM9*(P+DABS(M)+1.D0)
       IF(M.GT.-0.1D0)DUM9=DUM9-P
       IF(DUM9.LT.0.D0)DUM9=0.D0
       DUM9=DSQRT(2.D0)*DSQRT(DUM9)*2.D0
       DEM=DEM+DUM9*B(ISP,IIP,JP,KP)*B(IS,I,J,K)*ZNORR(NIP,NJPP1)*
     1ZNORR(NI,NJP1)*(DDP(NIP,NJPP1)*DDD(NI,NJP3)-DDP(NI,NJP3)*
     2DDD(NIP,NJPP1))/(XLAM*(NZP-NZ-2.D0))
       DUM9=P*(P+DABS(M))*2.D0
       IF(DUM9.LT.0.D0)DUM9= 0.D0
       DUM9= DSQRT(DUM9)*2.D0
       DEM=DEM+DUM9*C(ISP,IIP,JP,KP)*C(IS,I,J,K)*ZNORR(NIP,NJPP1)*
     1ZNORR(NI,NJP1)*(DDP(NIP,NJPP1)*DDD(NI,NJP3)-DDP(NI,NJP3)*DDD(NJP,
     2NJPP1))/(XLAM*(NZP-NZ-2.D0))
       DUM9= P+1.D0
       IF(M.GT.-0.1D0)DUM9=DUM9-1.D0
       DUM9=DUM9*(P+DABS(M))*2.D0
       IF(DUM9.LT.0.D0)DUM9= 0.D0
       DUM9=DSQRT(DUM9)*2.D0
       DEM=DEM+DUM9*D(ISP,IIP,JP,KP)*D(IS,I,J,K)*ZNORR(NIP,NJP)*
     1ZNORR(NI,NJ)*DDP(NIP,NJP)*DDD(NI,NJP2)/(XLAM*(NZP-NZ-2.D0))
       DUM9= P+1.D0
       IF(M.GT.-0.1D0)DUM9=DUM9-1.D0
       DUM9=DUM9*(P+DABS(M))
       IF(M.GT.-0.1D0)DUM9=DUM9+P
       IF(DUM9.LT.0.D0)DUM9=0.D0
       DUM9=DSQRT(DUM9)*(-2.D0)
       DUM9=P*(P+DABS(M))
       IF(DUM9.LT.0.D0)DUM9= 0.D0
       DUM9=DSQRT(DUM9)*(-2.D0)
       AM(IL,JL)=AM(IL,JL)-KAPPA*H*MU*DEM
       GO TO 415
  887 CONTINUE
       DUM9=NZP1*NZP2*P*(P+DABS(M))
       IF(DUM9.LT.0.D0)DUM9= 0.D0
       DUM9= 4.D0*(-X)*DSQRT(DUM9)
       DEM=DUM9*A(ISP,IIP,JP,KP)*A(IS,I,J,K)*ZNORR(NIP,NJP)*ZNORR(NI,NJP2
     1)*DDD(NIP,NJP)*DDD(NI,NJP2)/(NZP-NZ-2.D0)
       DUM9= P+1.D0
       IF(M.GT.-0.1D0)DUM9=DUM9-1.D0
       DUM9=DUM9*(P+DABS(M))*2.D0
       IF(DUM9.LT.0.D0)DUM9= 0.D0
       DUM9= 2.D0*DSQRT(DUM9)
       DEM=DEM+DUM9*B(ISP,IIP,JP,KP)*B(IS,I,J,K)*ZNORR(NIP,NJPP1)*
     1ZNORR(NI,NJP1)*DDD(NIP,NJPP1)*DDD(NI,NJP2)/(XLAM*(NZP-NZ-2.D0))
       DUM9= P*(P+DABS(M))*2.D0
       DUM9= 2.D0*DSQRT(DUM9)
```

```
      DEM=DEM+DUM9*C(ISP,IIP,JP,KP)*C(IS,I,J,K)*ZNORR(NIP,NJPP1)*
     1ZNORR(NI,NJP1)*DDD(NIP,NJP)*DDD(NI,NJP2)/(XLAM*(NZP-NZ-2.D0))
       DUM9= P+1.D0
      IF(M.GT.-0.1D0)DUM9=DUM9-1.D0
      DUM9=DUM9*NZP1*NZP2*(P+DABS(M)+1.D0)
      IF(DUM9.LT.0.D0)DUM9= 0.D0
      DUM9=-4.D0*DSQRT(DUM9)*(-X)
      DEM=DEM+DUM9*D(ISP,IIP,JP,KP)*D(IS,I,J,K)*ZNORR(NIP,NJP)*
     1ZNORR(NI,NJ)*DDD(NIP,NJP)*DDD(NI,NJP2)/(NZP-NZ-2.D0)
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*MU*DEM
  415 CONTINUE
  316 CONTINUE
C     RESTORE P,M,NZ VALUES
      IF(ISP.EQ.2.OR.ISP.EQ.3)INZP=INZP+1
      IF(ISP.EQ.2.OR.ISP.EQ.4)IMP=IMP+1
      IF(ISP.EQ.4.AND.IMP.LE.0)IPP=IPP+1
      IF(ISP.EQ.2.AND.IMP.LE.0)IPP=IPP+1
      IF(IS.EQ.2.OR.IS.EQ.3)INZ=INZ+1
      IF(IS.EQ.2.OR.IS.EQ.4)IM=IM+1
      IF(IS.EQ.4.AND.IM.LE.0)IP=IP+1
      IF(IS.EQ.2.AND.IM.LE.0)IP=IP+1
      INZPP1=INZP+1
      IF(ISP.EQ.3.OR.ISP.EQ.2)NZP=NZZ(INZPP1)
      IF(ISP.EQ.2.OR.ISP.EQ.4)MP=MP+1.D0
      IF(ISP.EQ.4.AND.IMP.LE.0)PP=PP+1.D0
      IF(ISP.EQ.2.AND.IMP.LE.0)PP=PP+1.D0
      INZP1=INZ+1
      IF(IS.EQ.3.OR.IS.EQ.2)NZ=NZZ(INZP1)
      IF(IS.EQ.2.OR.IS.EQ.4)M=M+1.D0
      IF(IS.EQ.4.AND.IM.LE.0)P=P+1.D0
      IF(IS.EQ.2.AND.IM.LE.0)P=P+1.D0
  317 CONTINUE
      IL=IL+1
      ISP=ISP+1
      IF(ISP.LE.4)GO TO 235
      NZPTE=INZP
      TEST=MAXP-NZPTE
      TEST=DABS(TEST)
      IF(TEST.LT. 1.D-03)GO TO 240
      INZP=INZP+2
      INZPP1=INZP+1
      NZP=NZZ(INZPP1)
      GO TO 230
  240 TEST=NTP-MP
      TEST=DABS(TEST)
      IF(TEST.LT. 1.D-03)GO TO 250
      MP=MP+1.D0
      IMP=IMP+1
      GO TO 220
  250 NTP=NTP+1.D0
      INP=INP+1
      IF(INP.LE.NSHEL)GO TO 210
  139 CONTINUE
      NZTE=INZ
      TEST=MAX-NZTE
      TEST=DABS(TEST)
      IF(TEST.LT.1.D-03)GO TO 140
      INZ=INZ+2
      INZP1=INZ+1
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      NZ=NZZ(INZP1)
      GO TO 130
  140 TEST=NT-M
      TEST=DABS(TEST)
      IF(TEST.LT. 1.D-03)GO TO 150
      M=M+1.DO
      IM=IM+1
      GO TO 120
  150 NT=NT+1.DO
      IN=IN+1
      IF(IN.LE.NSHEL)GO TO 110
      WRITE(6,885)
  885 FORMAT(1X,'POW')
      KO= 0.DO
      EPS= 1.D-12
      ABSCNV=.TRUE.
      TRD=.FALSE.
      FAIL=23
      WRITE(6,123)((AM(IL,JL),IL=1,16),JL=1,16)
  123 FORMAT(1X,5D22.15)
      CALL SYMQR(AM,DL,EL,KO,N,NA,EPS,ABSCNV,VEC,TRD,FAIL)
      DO 124 I=1,N
  124 DL(I)=DL(I)-MC2
      WRITE(6,2)(DL(I),I=1,N),(EL(I),I=1,N)
    2 FORMAT(1X,104(5D22.15,/,1X))
      WRITE(6,43)FAIL
   43 FORMAT(1X,I3)
      STOP
      END
      SUBROUTINE SYMQR(A,D,E,KO,N,NA,EPS,ABSCNV,VEC,TRD,FAIL)
C
C
C     EXPLANATION OF THE PARAMETERS IN THE CALLING SEQUENCE.
C
C          A       A DOUBLE DIMENSIONED ARRAY,  IF THE MATRIX IS NOT
C                  INITIALLY TRIDIAGONAL, IT IS CONTAINED IN THE LOWER
C                   TRIANGLE OF A.  IF EIGENVECTORS ARE NOT REQUESTED
C                  THE LOWER TRIANGLE OF A IS DESTROYED WHILE THE
C                  ELEMENTS ABOVE THE DIAGONAL ARE LEFT UNDISTURBED.
C                  IF EIGENVECTORS ARE REQUESTED. THEY ARE RETURNED IN THE
C                  COLUMNS OF A
C
C     D            A SINGLY SUBSCRIPTED ARRAY.  IF THE MATRIX IS
C                  INITIALLY TRIDIAGONAL, D CONTAINS ITS DIAGONAL
C                  ELEMENTS.  ON RETURN D CONTAINS THE EIGENVALUES OF
C                  THE MATRIX
C
C     E            A SINGLY SUBSCRIPTED ARRAY.  IF THE MATRIX IS
C                  INITIALLY TRIDIAGONAL, E CONTAINS ITS OFF-DIAGONAL
C                  ELEMENTS.UPON RETURN E(I) CONTAINS THE NUMBER OF
C                  ITERATIONS REQUIRED TO COMPUTE THE APPROXIMATE
C                  EIGENVALUE D(I)
C
C     KO           A REAL VARIABLE CONTAING AN INITIAL ORIGIN SHIFT TO
C                  BE USED UNTIL THE COMPUTED SHIFTS SETTLE DOWN.
C
C     N            AN INTEGER VARIABLE CONTAINING THE ORDER OF THE
C                  MATRIX.
C
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C     NA          AN INTEGER VARIABLE CONTAINING THE FIRST DIMENSION
C                 OF THE ARRAY A.
C
C     EPS         A REAL VARIABLE CONTAING A CONVERGENCE TOLERANCE
C
C     ABSCNV A LOGICAL VARIABLE CONTAINING THE VALUE .TRUE. IF
C                 THE ABSOLUTE CONVERGENCE CRITERION IS TO BE USED
C                 OR THE VALUE .FALSE. IF THE RELATIVE CRITERION
C                 IS TO BE USED.
C
C     VEC         A LOGICAL VARIABLE CONTAING THE VALUE.TRUE. IF
C                 EIGENVECTORS ARE TO BE COMPUTED AND RETURNED IN
C                 THE ARRAY A AND OTHERWISE CONTAINING THE VALUE .FALSE<<
C
C     TRD         A LOGICAL VARIABLE CONTAING THE VALUE .TRUE.
C                 IF THE MATRIS IS TRIDIAGONAL AND LOCATED IN THE ARRAYS
C                 D AND E AND OTHERWISE  CONTAINING THE VALJE .FALSE..
C
C     FAIL        AB INTEGER VARIABLE CONTAING A ERROR SIGNAL.
C     ON RETURN THE EIGENVALUES IN D(FAIL+1).....D(N)
C                 AND THEIR CORRESPONDING EIGENVECTORS MAY BE PRESUMED
C                 ACCURATE.
C
C
      REAL*8
     1A(N,N),D(N),E(N),KO,K1,K2,<,EPS,S2,CON,NINF,TEST,CB,CC,CD,
     2C,S,TEMP,P,PP,Q,QQ,NORM,R,TITTER,SUM,SUM1,MAX
      REAL*8 DMAX1,DMIN1
      REAL*8 DABS
      REAL*8 AGD
      REAL*8 DSQRT
      REAL*8 DSIGN
      INTEGER FAIL,SINCOS,RETURN
      LOGICAL
     1ABSCNV,VEC,TRD,SHFT
      TITTER= 50.
      NM1= N-1
      NM2=N-2
      NINF=0.
      ASSIGN 500 TO SINCOS
C
C      SIGNAL ERROR IF N IS NOT POSITIVE.
C
      IF(N.GT.0) GO TO 1
      FAIL = -1
      RETURN
C
C     SPECIAL TREATMENT FOR A MATRIX OF ORDER ONE.
C
    1 IF(N.GT.1) GO TO 5
      IF(.NOT.TRD) D(1) = A(1,1)
      IF(VEC) A(1,1) = 1.
      FAIL =0
      RETURN
C
C     IF THE MATRIX IS TRIDIAGONAL, SKIP THE REDUCTION.
C
    5 IF(TRD) GO TO 100
      IF(N.EQ.2) GO TO 80
```

```
C
C     REDUCE THE MATRIX TO TRIDIAGONAL FORM BY HOUSEHOLDERS METHOD.
C
      DO 70 L=1,NM2
      L1 = L+1
      D(L) = A(L,L)
      MAX = 0.
      DO 10 I=L1,N
      AGD= A(I,L)
   10 MAX= DMAX1(MAX,DABS(AGD))
      IF(MAX.NE.0.) GO TO 13
      E(L) = 0.
      A(L,L) = 1.
      GO TO 70
   13 SUM = 0.
      DO 17 I=L1,N
      A(I,L) = A(I,L)/MAX
   17 SUM= SUM+ A(I,L)**2
      S2 = SUM
      S2= DSQRT(S2)
      IF(A(L1,L) .LT. 0.) S2 = -S2
      E(L) = -S2*MAX
      A(L1,L) = A(L1,L) +S2
      A(L,L) = S2*A(L1,L)
      SUM1 = 0.
      DO 50 I=L1,N
      SUM = 0.
      DO 20 J=L1,I
   20 SUM = SUM + A(I,J)*A(J,L)
      IF(I.EQ.N) GO TO 40
      I1 = I+1
      DO 30 J=I1,N
   30 SUM = SUM + A(J,L)*A(J,I)
   40 E(I) = SUM/A(L,L)
   50 SUM1 = SUM1 + A(I,L)*E(I)
      CON =  .5*SUM1/A(L,L)
      DO 60 I=L1,N
      E(I) =E(I) - CON*A(I,L)
      DO 60 J=L1,I
   60 A(I,J) = A(I,J) - A(I,L)*E(J) - A(J,L)*E(I)
   70 CONTINUE
   80 D(NM1) = A(NM1,NM1)
      D(N) = A(N,N)
      E(NM1) = A(N,NM1)
C
C     IF EIGENVECTORS ARE REQUIRED, INITIALIZE A.
C
  100 IF(.NOT.VEC) GO TO 180
C
C     IF THE MATRIX WAS TRIDIAGONAL, SET A EQUAL TO THE IDENTITY MATRIX.
C
      IF(.NOT.TRD .AND. N.NE.2) GO TO 130
      DO 120 I=1,N
      DO 110 J=1,N
  110 A(I,J) = 0.
  120 A(I,I) = 1.
      GO TO 180
C
C     IF THE MATRIX WAS NOT TRIDIAGONAL, MULTIPLY OUT THE
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```
C     TRANSFORMATIONS OBTAINED IN THE HOUSEHOLDER REDUCTION.
C
  130 A(N,N) = 1.
      A(NM1,NM1) = 1.
      A(NM1,N)= 0.
      A(N,NM1) = 0.
      DO 170 L=1,NM2
      LL=NM2-L+1
      LL1 = LL+1
      DO 140 I=LL1,N
      SUM= 0.
      DO 135 J=LL1,N
  135 SUM =SUM + A(J,LL)*A(J,I)
  140 A(LL,I) = SUM/A(LL,LL)
      DO 150 I=LL1,N
      DO 150 J=LL1,N
  150 A(I,J) = A(I,J) - A(I,LL)*A(LL,J)
      DO 160 I=LL1,N
      A(I,LL) = 0.
  160 A(LL,I) = 0.
  170 A(LL,LL) = 1.
C
C     IF AN ABSOLUTE CONVERGENCE CRITERION IS REQUESTED
C     (ABSCNV=.TRUE.), COMPUTE THE INFINITY NORM OF THE MATRIX.
C
  180 IF(.NOT.ABSCNV) GO TO 200
      NINF =DMAX1(DABS(D(1))+DABS(E(1)),DABS(D(N))+DABS(E(NM1)))
      IF(N.EQ.2) GO TO 200
      DO 190 I=2,NM1
  190 NINF = DMAX1(NINF,DABS(D(I))+DABS(E(I))+DABS(E(I-1)))
C
C     START THE QR ITERATION.
C
  200 NU =N
      NUM1 = N-1
      SHFT = .FALSE.
      K1= K0
      TEST = NINF*EPS
      E(N) = 0.
C
C     CHECK FOR CONVERGENCE AND LOCATE THE SUBMATRIX IN WHICH THE
C     QR STEP IS TO BE PERFORMED.
C
  210 DO 220 NNL=1,NUM1
      NL= NUM1-NNL+1
      IF(.NOT.ABSCNV) TEST = EPS*DMIN1(DABS(D(NL)),DABS(D(NL+1)))
      IF(DABS(E(NL)).LE.TEST)GO TO 230
  220 CONTINUE
      GO TO 240
  230 E(NL) = 0.
      NL= NL+1
      IF(NL .NE. NU) GO TO 240
      IF(NUM1 .EQ. 1) RETURN
      NU = NUM1
      NUM1 = NU-1
      GO TO 210
  240 E(NU)= E(NU)+1.
      IF(E(NU).LE.TITTER)GO TO 250
      FAIL = NU
```

```
      RETURN
C
C     CALCULATE THE SHIFT
C
  250 CB= (D(NUM1)-D(NU))/ 2.
      MAX= DMAX1(DABS(CB),DABS(E(NUM1)))
      CB=CB/MAX
      CC=(E(NUM1)/MAX)**2
      CD=DSQRT(CB**2 + CC)
      IF(CB .NE.0.) CD =DSIGN(CD,CB)
      K2 = D(NU) - MAX*CC/(CB+CD)
      IF(SHFT) GO TO 270
      IF(DABS(K2-K1) .LT.  .5*DABS(K2)) GO TO 260
      K1=K2
      K= K0
      GO TO 300
  260 SHFT= .TRUE.
  270 K = K2
C
C     PERFORM ONE QR STEP WITH SHIFT K ON ROWS AND COLUMNS
C     NL THROUGH NU
C
  300 P=D(NL)-K
      Q = E(NL)
      ASSIGN 310 TO RETURN
      GO TO SINCOS,(500)
  310 I=NL-1
  311 I=I+1
C
C     IF REQUIRED, ROTATE THE EIGENVECTORS.
C
      IF(.NOT.VEC) GO TO 330
      DO 320 J=1,N
      TEMP = C*A(J,I) + S*A(J,I+1)
      A(J,I+1) = -S*A(J,I) + C*A(J,I+1)
  320 A(J,I) = TEMP
C
C     PERFORM THE SIMILARITY TRANSFORMATION AND CALCULATE THE NEXT
C     ROTATION.
C
  330 D(I) = C*D(I) + S*E(I)
      TEMP = C*E(I) + S*D(I+1)
      D(I+1) = -S*E(I) + C*D(I+1)
      E(I) = -S*K
      D(I) = C*D(I) +S*TEMP
      IF(I .EQ.NUM1) GO TO 380
      IF(DABS(S).GT.DABS(C))GO TO 350
      R= S/C
      D(I+1) = -S*E(I) + C*D(I+1)
      P = D(I+1) - K
      Q=C*E(I+1)
      ASSIGN 340 TO RETURN
      GO TO SINCOS,(500)
  340 E(I) = R*NORM
      E(I+1)=Q
      GO TO 380
  350 P= C*E(I) + S*D(I+1)
      Q = S*E(I+1)
      D(I+1) = C*P/S + K
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```
      E(I+1) = C*E(I+1)
      ASSIGN 360 TO RETURN
      GO TO SINCOS,(500)
  360 E(I) = NORM
  380 IF(I.LT.NUM1)GO TO 311
      TEMP = C*E(NUM1) + S*D(NU)
      D(NU) = -S*E(NUM1) + C*D(NJ)
      E(NUM1) = TEMP
      GO TO 210
C
C     INTERNAL PROCEDURE TO CALCULATE THE ROTATION CORRESPONDING TO
C     THE VECTOR(P,Q).
C
  500 PP = DABS(P)
      QQ= DABS(Q)
      IF(QQ.GT.PP) GO TO 510
       NORM= PP*DSQRT( 1. + (QQ/PP)**2)
      GO TO 520
  510 IF(QQ .EQ. 0.) GO TO 530
      NORM=QQ*DSQRT( 1. + (PP/QQ)**2)
  520 C = P/NORM
      S= Q/NORM
      GO TO RETURN,(310,340,360)
  530 C=1.
      S = 0.
      NORM = 0.
      GO TO RETURN,(310,340,360)
      END
      FUNCTION ZNORM(NZ,X,ZO)
      REAL*8 ZNORM
      REAL*8 NZ,X,D,DPRPN,DP,DPN,XLAM,ZO
      REAL*8 DD
      REAL*8 DSQRT
      XLAM=-X/(DSQRT(2.DO)*ZO)
      ZNORM=DD(NZ,X)*DPRPN(NZ,X)-DP(NZ,X)*DPN(NZ,X)
      ZNORM=ZNORM**(-0.5DO)
      ZNORM= ZNORM*((DSQRT(2.DO)*XLAM/2.DO)**0.5)
      RETURN
      END
      FUNCTION DD(NZ,X)
      REAL*8 DD
      REAL*8 NZ,X,C1,C2,B1,B2,DGAMMA,DSQRT,DEXP,F11
      REAL*8 A,C,Z
      REAL*8 TEST,DABS
      REAL*8 DGAM
      REAL*8 TWO
      TWO= 2.
      B1= 0.5-0.5*NZ
      TEST=DABS(B1)
      IF(TEST.LT.1.D-13)C1= 0.DO
      IF(TEST.LT. 1.D-13)GO TO 2
      C1= 0.5
      C1=DGAM(C1)/DGAM(B1)
    2 CONTINUE
      B2= -0.5*NZ
       C2= -0.5
      TEST=DABS(B2)
      IF(TEST.LT. 1.D-13)C2= 0.DO
      IF(TEST.LT. 1.D-13)GO TO 1
```

```
      C2= DGAM(C2)/DGAM(B2)
      C2= C2*X/DSQRT(TWO)
    1 CONTINUE
      A=B2
      C= 0.5
      Z= 0.5*X*X
      DD=C1*F11(A,C,Z)
      A=B1
      C= 1.5
      DD=DD+C2*F11(A,C,Z)
      Z=-0.5*Z
      B2 =-B2
      DD=DD*( 2.D0**B2)*DEXP(Z)
      RETURN
      END
      FUNCTION F11(A,C,Z)
      REAL*8 F11
      REAL*8 A,C,Z,D,Y,N,EPS,DABS
      EPS= 1.D-13
      F11= 1.
      Y= 1.
      DO 1 I=1,100
      N=I
      D= N*(C+N-1.)
      Y= (A+N-1.)*Y/D
      Y= Y*Z
      IF(DABS(F11).LT. 1.D-13)GO TO 3
      D= Y/F11
      D= DABS(D)
      IF(D.LT.EPS) RETURN
    3 F11=F11+Y
    1 CONTINUE
      WRITE(6,2)
    2 FORMAT(1X,'ZAP')
      RETURN
      END
      FUNCTION DP(NZ,X)
      REAL*8 DP
      REAL*8 NZ,X,DD
      DP=-0.5*X*DD(NZ,X)+NZ*DD(NZ-1.,X)
      RETURN
      END
      FUNCTION DGAM(X)
      REAL*8 DGAM
      REAL*8 X,PI,DGAMMA,Y,DSIN,Z
      PI= 3.141592653589793
      IF(X.LT.+0.)GO TO 1
      DGAM= DGAMMA(X)
      RETURN
    1 Y= 1.-X
      Z= PI*X
      DGAM= PI/(DGAMMA(Y)*DSIN(Z))
      RETURN
      END
      FUNCTION DPRPN(NZ,X)
      REAL*8 DPRPN
      REAL*8 DP,NZ,X,EPS,A,B
      EPS= 1.D-05
      A=NZ+EPS
```

```
      B=NZ-EPS
      DPRPN=(DP(A,X)-DP(B,X))/(+2.D0*EPS)
      RETURN
      END
      FUNCTION DPN(NZ,X)
      REAL*8 DPN
      REAL*8 DD
      REAL*8 D,DA,NZ,X,EPS,A,B
      EPS= 1.D-05
      A= NZ+EPS
      B=NZ-EPS
      DPN=(DD(A,X)-DD(B,X))/(2.D0*EPS)
      RETURN
      END
//GO.SYSIN DD *
//
```

APPENDIX B

PROGRAM FOR Z0 = 0

This program does the same job as the one in APPENDIX A, except it is for $z_o = 0$.

```
$JOB
C      PROGRAM FOR Z0=0
C      THIS PROGRAM WAS WRITTEN BY EUGENE CHAFFIN AND CORRESPONDS TO
C      ZERO DEFORMATION.
       LOGICAL ABSCNV,VEC,TRD
       INTEGER FAIL
       REAL*8 AM(224,224)
       REAL*8 DL(224),EL(224),K0,EPS
       REAL*8 NZZ(7),NT,TEST
       REAL*8 A(4,3,11,6),B(4,3,11,6),C(4,3,11,6),D(4,3,11,6)
       REAL*8 MC2,E,F,G,H,DSQRT,DABS,DUM,DENOM,DEM
       REAL*8 EN,FN,P,M,NZ
       REAL*8 KAPPA,MU,NTP,PP,MP,NZP,MAXP,DUM2,DUM3,DUM4,DUM5,DUM6,DUM7,
      1DUM8,DUM9
       NSHEL=5
       VEC=.FALSE.
       LLL= 224
       N= 224
       NA=224
       K0= 0.D0
       EPS= 1.D-12
       ABSCNV=.TRUE.
       TRD=.FALSE.
       FAIL=23
       H= 7.03D0
       MC2= 938.256D0
       MU= 0.65
       KAPPA= 0.0577
       NZZ(1)= 0.D0
       NZZ(2)= 1.D0
       NZZ(3)= 2.D0
       NZZ(4)= 3.D0
       NZZ(5)= 4.D0
       NZZ(6)= 5.D0
       NZZ(7)= 6.D0
       L=0
       DO 500 LL=1,LLL
       DO 500 LP=1,LLL
       AM(LL,LP)= 0.D0
  500  CONTINUE
       IN=0
       NT= 0.D0
   10  M=-NT
       IM=-IN
   20  MAX=NT-DABS(M)
       IEVEN=IN-IABS(IM)
       IF(IEVEN.EQ.0)INZ=0
       IF(IEVEN.EQ.0)GO TO 29
       IEVEN=(-1)**IEVEN
       IF(IEVEN.LT.0)INZ=1
       IF(IEVEN.GT.0)INZ=0
   29  CONTINUE
       INZP1=INZ+1
       NZ=NZZ(INZP1)
   30  P=(NT-NZ-DABS(M))/2.D0
       IP=(IN-INZ-IABS(IM))/2
       IF(M.LT.-0.1D0)J=IABS(IM)+6
       IF(M.GT.-0.1D0)J=IM+1
       I=IP+1
```

```
      K=INZ+1
    1 E= 1.D0+2.D0*(H/MC2)*( 2.D0*P+DABS(M)+NZ+2.5D0)+H*H*(M*M+M+1.25D0
     1)/(MC2*MC2)
      G= 1.D0+2.D0*(H/MC2)*( 2.D0*P+DABS(M)+1.5D0)+H*H*(M*M+M+0.25D0)/
     1(MC2*MC2)
      G=DSQRT(G)
      E= E-2.D0*(H/MC2)*G
      E= MC2*DSQRT(E)
      L=L+1
      AM(L,L)=E-H*H*(M*M+M+0.25D0)/( 2.D0*MC2)
      AM(L,L)=AM(L,L)+H*H*(2.D0*P+DABS(M)+1.5D0)/MC2
      AM(L,L)=AM(L,L)+KAPPA*H*MU* 0.5D0*NT*(NT+3.D0)
    3 A(1,I,J,K)= 1.D0
      DJM= 2.D0*(P+(M+DABS(M))/2.D0+1.D0)*(NZ+1.D0)
      DUM=-4.D0*H*H*MC2*DSQRT(DUM)
      DENOM=(((MC2-H*(M-0.5D0))**2+4.D0*H*MC2*(P+(M+DABS(M))/2.D0
     1+NZ/2.D0+1.5D0)-E*E)*(-MC2-E+H*(M+1.5D0))-8.D0*MC2*H*H*(P+(
     2M+DABS(M))/2.D0+1.D0))
      B(1,I,J,K)= DUM/DENOM
      IF(M.LT.-0.1D0)B(1,I,J,K)=-B(1,I,J,K)
      DUM= 2.D0*(NZ+1.D0)*MC2*H
      DJM=DSQRT(DUM)/(-MC2-E+H*(M+1.5D0))
      C(1,I,J,K)=-DJM*(1.D0+8.D0*MC2*H*H*(P+(M+DABS(M))/2.D0+1.D0)/DENOM
     1)
      DUM=(P+(M+DABS(M))/2.D0+1.D0)*MC2*H
      DUM= -2.D0*DSQRT(DUM)/(-MC2-E+H*(M-0.5D0))
      IF(M.LT. -0.1D0)DUM=-DUM
      D(1,I,J,K)= DUM*(1.D0-4.D0*MC2*H*H*(NZ+1.D0)/DENOM)
      DUM= 1.D0+B(1,I,J,K)**2+C(1,I,J,K)**2+D(1,I,J,K)**2
      DUM=DSQRT(DUM)
      A(1,I,J,K)= 1.D0/DUM
      B(1,I,J,K)= B(1,I,J,K)/DUM
      C(1,I,J,K)=C(1,I,J,K)/DUM
      D(1,I,J,K)=D(1,I,J,K)/DUM
      IF(IM.LE.0)P=P-1.D0
      M=M-1.D0
      IF(INZ.EQ.0)NZ=-1.D0
      IF(INZ.GT.0)NZ=NZZ(INZ)
      E= 1.D0+2.D0*(H/MC2)*( 2.D0*P+DABS(M)+NZ+2.5D0)+H*H*(M*M+M+1.25D0
     1)/(MC2*MC2)
      G= 1.D0+2.D0*(H/MC2)*( 2.D0*P+DABS(M)+1.5D0)+H*H*(M*M+M+0.25D0)/
     1(MC2*MC2)
      G=DSQRT(G)
      F= E+2.D0*(H/MC2)*G
      F=MC2*DSQRT(F)
    4 B(2,I,J,K)=-1.D0
      IF(M.LT.-0.1D0)B(2,I,J,K)=-B(2,I,J,K)
      DJM= 2.D0*(P+(M+DABS(M))/2.D0+1.D0)*(NZ+1.D0)
      DUM=-4.D0*H*H*MC2*DSQRT(DUM)
      DEM=(((MC2-H*(M+1.5D0))**2+4.D0*H*MC2*(P+(M+DABS(M))/2.D0+NZ/2.D0
     1+1.5D0)-F*F)*(-MC2-F+H*(M-0.5D0))+8.D0*MC2*H*H*(P+(M+DABS(M))/2.D0
     2+1.D0))
      A(2,I,J,K)=-DUM/DEM
      DUM= (P+(M+DABS(M))/2.D0+1.D0)*MC2*H
      DUM= -2.D0*DSQRT(DUM)/(-MC2-F+H*(M+1.5D0))
      C(2,I,J,K)= DUM*(1.D0+4.D0*MC2*H*H*(NZ+1.D0)/DEM)
      DUM= 2.D0*(NZ+1.D0)*MC2*H
      DUM=  DSQRT(DUM)/(-MC2-F+H*(M-0.5D0))
      IF(M.LT. -0.1D0)DUM=-DUM
```

```
      AM(L,L)=FN+H*H*(M*M+M+0.25D0)/( 2.D0*MC2)
      AM(L,L)=AM(L,L)+H*H*(2.D0*P+DABS(M)+1.5D0)/MC2
      AM(L,L)=AM(L,L)+KAPPA*H*MU* 0.5D0*NT*(NT+3.D0)
    5 D(4,I,J,K)=-1.D0
      IF(M.LT.-0.1D0)D(4,I,J,K)=-D(4,I,J,K)
      DUM= 2.D0*(P+(M+DABS(M))/2.D0+1.D0)*(NZ+1.D0)
       DUM= 4.D0*H*H*MC2*DSQRT(DJM)
      DEM  =(((MC2-H*(M+1.5D0))**2+4.D0*H*MC2*(P+(M+DABS(M))/2.D0
     1+NZ/2.D0+1.5D0)-FN*FN)*( MC2-FN-H*(M-0.5D0))-8.D0*MC2*H*H*(P+(
     2M+DABS(M))/2.D0+1.D0))
      C(4,I,J,K)= DUM/DEM
      DUM= 2.D0*(NZ+1.D0)*MC2*H
      DUM=DSQRT(DUM)/( MC2-FN-H*(M-0.5D0))
      DUM=-DUM
      IF(M.GT.-0.1D0)DUM=-DUM
      B(4,I,J,K)= DUM*( 1.D0+8.D0*MC2*H*H*(P+(M+DABS(M))/2.D0+1.D0)/DEM)
      DUM= (P+(M+DABS(M))/2.D0+1.D0)*MC2*H
      DUM=-2.D0*DSQRT(DUM)/( MC2-FN-H*(M+1.5D0))
      DUM=-DUM
      A(4,I,J,K)=DUM*(1.D0-4.D0*MC2*H*H*(NZ+1.D0)/DEM)
      DUM= A(4,I,J,K)**2+B(4,I,J,K)**2+C(4,I,J,K)**2+1.D0
      DUM=DSQRT(DUM)
      A(4,I,J,K)=A(4,I,J,K)/DUM
      B(4,I,J,K)= B(4,I,J,K)/DUM
      C(4,I,J,K)=C(4,I,J,K)/DUM
      D(4,I,J,K)=D(4,I,J,K)/DUM
    7 CONTINUE
      M=M+1.D0
      IF(IM.LE.0)P=P+1.D0
      TEST=MAX-NZ
      TEST=DABS(TEST)
      IF(TEST.LT. 1.D-03)GO TO 40
      INZ=INZ+2
      INZP1=INZ+1
      NZ=NZZ(INZP1)
      GO TO 30
   40 TEST=NT-M
      TEST=DABS(TEST)
      IF(TEST.LT. 1.D-03)GO TO 50
      M=M+1.D0
      IM=IM+1
      GO TO 20
   50 NT=NT+1.D0
      IN=IN+1
      IF(IN.LE.NSHEL)GO TO 10
      IL=0
      JL=0
      IN=0
      NT= 0.D0
  110 M=-NT
      IM=-IN
  120 MAX=NT-DABS(M)
      IEVEN=IN-IABS(IM)
      IF(IEVEN.EQ.0)INZ=0
      IF(IEVEN.EQ.0)GO TO 129
      IEVEN=(-1)**IEVEN
      IF(IEVEN.LT.0)INZ=1
      IF(IEVEN.GT.0)INZ=0
  129 CONTINUE
```

```
      D(2,I,J,K)= DUM*(1.D0-8.D0*MC2*H*H*(P+(M+DABS(M))/2.D0+1.D0)/DEM)
      DJM= A(2,I,J,K)**2+1.D0+C(2,I,J,K)**2+D(2,I,J,K)**2
      DUM=DSQRT(DUM)
      A(2,I,J,K)=A(2,I,J,K)/DUM
      B(2,I,J,K)=B(2,I,J,K)/DUM
      C(2,I,J,K)=C(2,I,J,K)/DUM
      D(2,I,J,K)=D(2,I,J,K)/DUM
      L=L+1
      AM(L,L)=F-H*H*(M*M+M+0.25D0)/( 2.D0*MC2)
      AM(L,L)=AM(L,L)-H*H*(2.D0*P+DABS(M)+1.5D0)/MC2
      AM(L,L)=AM(L,L)+KAPPA*H*MJ* 0.5D0*NT*(NT+3.D0)
      M=M+1.D0
      IF(IM.LE.0)P=P+1.D0
      E= 1.D0+2.D0*(H/MC2)*( 2.D0*P+DABS(M)+NZ+2.5D0)+H*H*(M*M+M+1.25D0
     1)/(MC2*MC2)
      G= 1.D0+2.D0*(H/MC2)*( 2.D0*P+DABS(M)+1.5D0)+H*H*(M*M+M+0.25D0)/
     1(MC2*MC2)
      G=DSQRT(G)
      E=E-2.D0*(H/MC2)*G
      E= MC2*DSQRT(E)
      EN=-E
      L=L+1
      AM(L,L)=EN+H*H*(M*M+M+0.25D0)/( 2.D0*MC2)
      AM(L,L)=AM(L,L)-H*H*(2.D0*P+DABS(M)+1.5D0)/MC2
      AM(L,L)=AM(L,L)+KAPPA*H*MJ* 0.5D0*NT*(NT+3.D0)
    5 C(3,I,J,K)=-1.D0
      DUM= 2.D0*(P+(M+DABS(M))/2.D0+1.D0)*(NZ+1.D0)
      DENOM=(((MC2-H*(M-0.5D0))**2+4.D0*H*MC2*(P+(M+DABS(M))/2.D0
     1+NZ/2.D0+1.5D0)-EN*EN)*( MC2-EN-H*(M+1.5D0))+8.D0*MC2*H*H*(P+(
     2M+DABS(M))/2.D0+1.D0))
      D(3,I,J,K)= DUM/DENOM
       DUM= 4.D0*H*H*MC2*DSQRT(DUM)
      IF(M.LT.-0.1D0)D(3,I,J,K)=-D(3,I,J,K)
      DUM= 2.D0*(NZ+1.D0)*MC2*H
      DUM= DSQRT(DUM)/( MC2-EN-H*(M+1.5D0))
      A(3,I,J,K)= DJM*( 1.D0-8.D0*MC2*H*H*(P+(M+DABS(M))/2.D0+1.D0)
     1/DENOM)
      DUM= (P+(M+DABS(M))/2.D0+1.D0)*MC2*H
      DUM=  2.D0*DSQRT(DUM)/( MC2-EN-H*(M-0.5D0))
      IF(M.GT.-0.1D0)DUM=-DUM
      B(3,I,J,K)= DUM*( 1.D0+4.D0*MC2*H*H*(NZ+1.D0)/DENOM)
      DUM= A(3,I,J,K)**2+B(3,I,J,K)**2+1.D0+D(3,I,J,K)**2
      DUM=DSQRT(DUM)
      A(3,I,J,K)=A(3,I,J,K)/DUM
      B(3,I,J,K)=B(3,I,J,K)/DUM
      C(3,I,J,K)=C(3,I,J,K)/DUM
      D(3,I,J,K)=D(3,I,J,K)/DUM
      IF(IM.LE.0)P=P-1.D0
      M=M-1.D0
      NZ=NZZ(INZP1)
      E= 1.D0+2.D0*(H/MC2)*( 2.D0*P+DABS(M)+NZ+2.5D0)+H*H*(M*M+M+1.25D0
     1)/(MC2*MC2)
      G= 1.D0+2.D0*(H/MC2)*( 2.D0*P+DABS(M)+1.5D0)+H*H*(M*M+M+0.25D0)/
     1(MC2*MC2)
      G=DSQRT(G)
      F=E+2.D0*(H/MC2)*G
      F=MC2*DSQRT(F)
      FN=-F
      L=L+1
```

```
      INZP1=INZ+1
      NZ=NZZ(INZP1)
  130 P=(NT-NZ-DABS(M))/2.D0
      IP=(IN-INZ-IABS(IM))/2
      IF(M.LT.-0.1D0)J=IABS(IM)+6
      IF(M.GT.-0.1D0)J=IM+1
      I=IP+1
      K=INZ+1
      DO 139 IS=1,4
      JL=JL+1
      IL=JL
      NTP=NT
      INP=IN
      PP=P
      MP=M
      NZP=NZ
      MAXP=MAX
      INZP=INZ
      IMP=IM
      IPP=IP
      ISP=IS
      IIP=I
      JP=J
      KP=K
      GO TO 235
  210 MP=-NTP
      IMP=-INP
  220 MAXP=NTP-DABS(MP)
      IEVENP=INP-IABS(IMP)
      IF(IEVENP.EQ.0)INZP=0
      IF(IEVENP.EQ.0)GO TO 229
      IEVENP=(-1)**IEVENP
      IF(IEVENP.LT.0)INZP=1
      IF(IEVENP.GT.0)INZP=0
  229 CONTINUE
      INZPP1=INZP+1
      NZP=NZZ(INZPP1)
  230 PP=(NTP-NZP-DABS(MP))/2.D0
      IPP=(INP-INZP-IABS(IMP))/2
      IF(MP.LT.-0.1D0)JP=IABS(IMP)+6
      IF(MP.GT.-0.1D0)JP=IMP+1
      IIP=IPP+1
      KP=INZP+1
      ISP= 1
  235 CONTINUE
      IF(IS.EQ.2.AND.IM.LE.0)P=P-1.D0
      IF(IS.EQ.4.AND.IM.LE.0)P=P-1.D0
      IF(IS.EQ.2.OR.IS.EQ.4)M=M-1.D0
      IF(IS.EQ.2.AND.INZ.EQ.0)NZ=-1.D0
      IF(IS.EQ.3.AND.INZ.EQ.0)NZ=-1.D0
      IF(IS.EQ.2.AND.INZ.GT.0)NZ=NZZ(INZ)
      IF(IS.EQ.3.AND.INZ.GT.0)NZ=NZZ(INZ)
      IF(ISP.EQ.2.AND.IMP.LE.0)PP=PP-1.D0
      IF(ISP.EQ.4.AND.IMP.LE.0)PP=PP-1.D0
      IF(ISP.EQ.2.OR.ISP.EQ.4)MP=MP-1.D0
      IF(ISP.EQ.2.AND.INZP.EQ.0)NZP=-1.D0
      IF(ISP.EQ.2.AND.INZP.GT.0)NZP=NZZ(INZP)
      IF(ISP.EQ.3.AND.INZP.EQ.0)NZP=-1.D0
      IF(ISP.EQ.3.AND.INZP.GT.0)NZP=NZZ(INZP)
```

```
      IF(IS.EQ.2.AND.IM.LE.0)IP=IP-1
      IF(IS.EQ.4.AND.IM.LE.0)IP=IP-1
      IF(IS.EQ.2.OR.IS.EQ.4)IM=IM-1
      IF(IS.EQ.2.OR.IS.EQ.3)INZ=INZ-1
      IF(ISP.EQ.2.AND.IMP.LE.0)IPP=IPP-1
      IF(ISP.EQ.4.AND.IMP.LE.0)IPP=IPP-1
      IF(ISP.EQ.2.OR.ISP.EQ.4)IMP=IMP-1
      IF(ISP.EQ.2.OR.ISP.EQ.3)INZP=INZP-1
      DUM=2.D0*(NZ+1.D0)*(P+(M+DABS(M))/2.D0+1.D0)
      DUM=DSQRT(DUM)
      IF(M.GT.-0.1D0)DUM=-DUM
      IF(INZ.NE.INZP.OR.IP.NE.IPP.OR.IM.NE.IMP)GO TO 401
C     DIAGONAL AND (SPIN DOWN,SPIN UP), ETC. TYPE ELEMENTS OF L.S
      DEM=A(ISP,IIP,JP,KP)*A(IS,I,J,K)*M-B(ISP,IIP,JP,KP)*B(IS,I,J,K)*(
     1M+1.D0)+C(ISP,IIP,JP,KP)*C(IS,I,J,K)*M-D(ISP,IIP,JP,KP)*
     2D(IS,I,J,K)*(M+1.D0)+C(ISP,IIP,JP,KP)*D(IS,I,J,K)*DUM+D(ISP,IIP,
     3JP,KP)*C(IS,I,J,K)*DUM
      DEM= 0.5*DEM
      DEM= KAPPA*H*2.D0*DEM
      AM(IL,JL)=AM(IL,JL)-DEM
C     DIAGONAL AND(SPIN DOWN,SPIN UP), ETC. TYPE ELEMENTS OF L.L
      DEM=A(ISP,IIP,JP,KP)*A(IS,I,J,K)*(M*M+NZ*(2.D0*P+DABS(M)+2.D0)
     1+(NZ+1.D0)*(2.D0*P+DABS(M)))+B(ISP,IIP,JP,KP)*B(IS,I,J,K)*((M+1.D0
     2)*(M+1.D0)+(NZ+1.D0)*(2.D0*P+DABS(M)+3.D0)+(NZ+2.D0)*(2.D0*P+
     3DABS(M)+1.D0)) +C(ISP,IIP,JP,KP)*C(IS,I,J,K)*(M*M+(NZ+1.D0)*(2.D0
     4*P+DABS(M)+2.D0)+(NZ+2.D0)*(2.D0*P+DABS(M)))+D(ISP,IIP,JP,KP)*
     5D(IS,I,J,K)*((M+1.D0)*(M+1.D0)+NZ*(2.D0*P+DABS(M)+3.D0)+(NZ+1.D0)
     6*(2.D0*P+DABS(M)+1.D0))
      DEM=KAPPA*MU*H*DEM
      AM(IL,JL)=AM(IL,JL)-DEM
      GO TO 316
  401 CONTINUE
C     PP,P  MP,M  MZP,NZ+2  TERM OF L.S
      DUM2= 2.D0*(NZ+2.D0)*(P+(M+DABS(M))/2.D0+1.D0)
      IF(DUM2.LT.0.D0)DUM2= 0.D0
      DUM2=DSQRT(DUM2)
      IF(M.GT.-0.1D0)DUM2=-DUM2
      IF(IP.NE.IPP.OR.IM.NE.IMP)GO TO 405
      INZP2=INZ+2
      IF(INZP.NE.INZP2)GO TO 403
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*A(ISP,IIP,JP,KP)*B(IS,I,J,K)*DUM2
      GO TO 316
  403 CONTINUE
C     PP,P MP,M MZP,NZ-2 TERM OF L.S
      DUM3= 2.D0*NZ*(P+(M+DABS(M))/2.D0+1.D0)
      IF(DUM3.LT.0.D0)DUM3= 0.D0
      DUM3=DSQRT(DUM3)
      IF(M.GT.-0.1D0)DUM3=-DUM3
      INZM2=INZ-2
      IF(INZP.NE.INZM2)GO TO 405
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*B(ISP,IIP,JP,KP)*A(IS,I,J,K)*DUM3
      GO TO 316
  405 CONTINUE
C     PP,P-1 MP,M MZP,NZ TERM OF L.S
      IPM1=IP-1
      IF(IPP.NE.IPM1.OR.IMP.NE.IM.OR.INZ.NE.INZP)GO TO 407
      DUM4= 2.D0*(NZ+1.D0)*(P+(DABS(M)-M)/2.D0)
      IF(DUM4.LT.0.D0)DUM4= 0.D0
      DUM4= DSQRT(DUM4)
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      IF(M.GT.-0.1D0)DJM4=-DJM4
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*B(ISP,IIP,JP,KP)*A(IS,I,J,K)*DJM4
      GO TO 316
  407 CONTINUE
C     PP,P+1 MP,M NZP,NZ TERM OF L .S
      IPP1=IP+1
      IF(IPP.NE.IPP1.OR.IMP.NE.IM.OR.INZ.NE.INZP)GO TO 409
      DUM5= 2.D0*(NZ+1.D0)*(P+(DABS(M)-M)/2.D0+1.D0)
      IF(DUM5.LT.0.D0)DUM5= 0.D0
      DUM5=DSQRT(DUM5)
      IF(M.GT.-0.1D0)DUM5=-DUM5
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*A(ISP,IIP,JP,KP)*B(IS,I,J,K)*DUM5
  409 CONTINUE
C     PP,P+1 MP,M NZP,NZ-2 TERM OF L.S
      IPP1=IP+1
      INZM2=INZ-2
      IF(IPP.NE.IPP1.OR.INZP.NE.INZM2.OR.IMP.NE.IM)GO TO 411
      DUM6= 2.D0*NZ*(P+(DABS(M)-M)/2.D0+1.D0)
      IF(DUM6.LT.0.D0)DUM6= 0.D0
      DUM6=DSQRT(DUM6)
      IF(M.GT.-0.1D0)DUM6=-DJM6
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*C(ISP,IIP,JP,KP)*D(IS,I,J,K)*DJM6
C     PP,P+1 MP,M NZP,NZ-2  AND  PP,P+1 MP,M NZP+1,NZ-1 TERMS OF L.L
      DUM7=NZ*(NZ-1.D0)*(P+1.D0)*(P+DABS(M)+1.D0)
      IF(DUM7.LT.0.D0)DUM7= 0.D0
      DUM7= 2.D0*DSQRT(DUM7)
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*MU*A(ISP,IIP,JP,KP)*A(IS,I,J,K)*DJM7
      DJM7=NZ*(NZ-1.D0)*(P+1.D0)*(P+DABS(M)+2.D0)
      IF(DUM7.LT.0.D0)DUM7= 0.D0
      DUM7= 2.D0*DSQRT(DUM7)
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*MU*D(ISP,IIP,JP,KP)*D(IS,I,J,K)*DJM7
      DUM7= NZ*(NZ+1.D0)*(P+1.D0)*(P+DABS(M)+2.D0)
      IF(DUM7.LT.0.D0)DUM7= 0.D0
      DJM7=  2.D0*DSQRT(DUM7)
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*MJ*B(ISP,IIP,JP,KP)*B(IS,I,J,K)*DUM7
      DUM7= NZ*(NZ+1.D0)*(P+1.D0)*(P+DABS(M)+1.D0)
      IF(DUM7.LT.0.D0)DUM7= 0.D0
      DUM7= 2.D0*DSQRT(DUM7)
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*MU*C(ISP,IIP,JP,KP)*C(IS,I,J,K)*DJM7
  411 CONTINUE
C     PP,P-1 MP,M NZP,NZ+2  TERM OF L.S
      IPM1=IP-1
      INZP2=INZ+2
      IF(IPP.NE.IPM1.OR.INZP.NE.INZP2.OR.IMP.NE.IM)GO TO 413
      DUM8= 2.D0*(NZ+2.D0)*(P+(DABS(M)-M)/2.D0)
      IF(DUM8.LT.0.D0)DUM8= 0.D0
      DUM8=DSQRT(DUM8)
      IF(M.GT.-0.1D0)DUM8=-DUM8
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*MU*D(ISP,IIP,JP,KP)*C(IS,I,J,K)*DUM8
C     PP,P-1 MP,M NZP,NZ+2 AND PP,P-1 MP,M NZP+1,NZ+3 TERMS OF L.L
      DUM9=(NZ+1.D0)*(NZ+2.D0)*P*(P+DABS(M))
      IF(DUM9.LT.0.D0)DUM9= 0.D0
      DUM9= 2.D0*DSQRT(DUM9)
      AM(IL,JL)= AM(IL,JL)-KAPPA*H*MJ*A(ISP,IIP,JP,KP)*A(IS,I,J,K)*DJM9
      DUM9=(NZ+2.D0)*(NZ+3.D0)*P*(P+DABS(M)+1.D0)
      IF(DUM9.LT.0.D0)DUM9= 0.D0
      DUM9= 2.D0*DSQRT(DUM9)
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*MU*B(ISP,IIP,JP,KP)*B(IS,I,J,K)*DJM9
      DJM9=(NZ+2.D0)*(NZ+3.D0)*P*(P+DABS(M))
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      IF(DUM9.LT.0.D0)DUM9= 0.D0
      DUM9= 2.D0*DSQRT(DUM9)
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*MU*C(ISP,IIP,JP,KP)*C(IS,I,J,K)*DUM9
      DUM9=(NZ+1.D0)*(NZ+2.D0)*P*(P+DABS(M)+1.D0)
      IF(DUM9.LT.0.D0)DUM9= 0.D0
      DUM9= 2.D0*DSQRT(DUM9)
      AM(IL,JL)=AM(IL,JL)-KAPPA*H*MU*D(ISP,IIP,JP,KP)*D(IS,I,J,K)*DUM9
  413 CONTINUE
  316 CONTINUE
C     RESTORE P,M,NZ VALUES
      IF(ISP.EQ.2.OR.ISP.EQ.3)INZP=INZP+1
      IF(ISP.EQ.2.OR.ISP.EQ.4)IMP=IMP+1
      IF(ISP.EQ.4.AND.IMP.LE.0)IPP=IPP+1
      IF(ISP.EQ.2.AND.IMP.LE.0)IPP=IPP+1
      IF(IS.EQ.2.OR.IS.EQ.3)INZ=INZ+1
      IF(IS.EQ.2.OR.IS.EQ.4)IM=IM+1
      IF(IS.EQ.4.AND.IM.LE.0)IP=IP+1
      IF(IS.EQ.2.AND.IM.LE.0)IP=IP+1
      INZPP1=INZP+1
      IF(ISP.EQ.3.OR.ISP.EQ.2)NZP=NZZ(INZPP1)
      IF(ISP.EQ.2.OR.ISP.EQ.4)MP=MP+1.D0
      IF(ISP.EQ.4.AND.IMP.LE.0)PP=PP+1.D0
      IF(ISP.EQ.2.AND.IMP.LE.0)PP=PP+1.D0
      INZP1=INZ+1
      IF(IS.EQ.3.OR.IS.EQ.2)NZ=NZZ(INZP1)
      IF(IS.EQ.2.OR.IS.EQ.4)M=M+1.D0
      IF(IS.EQ.4.AND.IM.LE.0)P=P+1.D0
      IF(IS.EQ.2.AND.IM.LE.0)P=P+1.D0
      IL=IL+1
      ISP=ISP+1
      IF(ISP.LE.4)GO TO 235
      TEST=MAXP-NZP
      TEST=DABS(TEST)
      IF(TEST.LT. 1.D-03)GO TO 240
      INZP=INZP+2
      INZPP1=INZP+1
      NZP=NZZ(INZPP1)
      GO TO 230
  240 TEST=NTP-MP
      TEST=DABS(TEST)
      IF(TEST.LT. 1.D-03)GO TO 250
      MP=MP+1.D0
      IMP=IMP+1
      GO TO 220
  250 NTP=NTP+1.D0
      INP=INP+1
      IF(INP.LE.NSHEL)GO TO 210
  139 CONTINUE
      TEST=MAX-NZ
      TEST=DABS(TEST)
      IF(TEST.LT.1.D-03)GO TO 140
      INZ=INZ+2
      INZP1=INZ+1
      NZ=NZZ(INZP1)
      GO TO 130
  140 TEST=NT-M
      TEST=DABS(TEST)
      IF(TEST.LT. 1.D-03)GO TO 150
      M=M+1.D0
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      IM=IM+1
      GO TO 120
  150 NT=NT+1.D0
      IN=IN+1
      IF(IN.LE.NSHEL)GO TO 110
      CALL SYMQR(AM,DL,EL,KO,N,NA,EPS,ABSCNV,VEC,TRD,FAIL)
      WRITE(6,2)(DL(I),I=1,224),(EL(I),I=1,224)
    2 FORMAT(1X,104(5D22.15,/,1X))
      WRITE(6,43)FAIL
   43 FORMAT(1X,I3)
      STOP
      END
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VITA

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Doctor of Philosophy

Thesis: A RELATIVISTIC MODEL FOR NUCLEAR FISSION

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